CRYSTALS OF THE *ESCHERICHIA COLI* MEMBRANE-ASSOCIATED GLYCOSYLTRANSFERASE (MurG) PROTEIN, ATOMIC COORDINATES AND THREE-DIMENSIONAL STRUCTURES THEREOF, ATOMIC COORDINATES AND THREE-DIMENSIONAL STRUCTURES OF BINDING DOMAINS THEREOF, IMAGES THEREOF, AND METHODS OF CRYSTALLIZING MurG PROTEINS, MODELS OF UDP-GLYCOSYLTRANSFERASES, MurG PROTEINS AND BINDING SITES, METHODS OF MAKING MODELS, METHODS OF USING MODELS OF MurG, COMPOUNDS THAT BIND, INHIBIT OR STIMULATE MurG PROTEINS, AND THERAPEUTIC COMPOSITIONS THEREOF

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FIELD OF THE INVENTION

The present invention relates to crystals of the *Escherichia coli* MurG, a membrane-associated UDP-glycosyltransferase involved in peptidoglycan biosynthesis. The present invention also relates to three-dimensional atomic coordinates of the MurG protein, three-dimensional structures of the protein, and images thereof. The present invention also relates to the atomic coordinates and three-dimensional structures of the α-carbon backbone of the MurG protein and images thereof. The present invention further relates to the atomic coordinates and three-dimensional structures of the α-carbon backbone and conserved amino acid residue sidechains of the MurG protein and images thereof. The present invention further relates to three-dimensional atomic coordinates of the donor nucleotide binding site, the acceptor binding site, and the membrane association site of the MurG protein, three-dimensional structures of the binding domains, and images thereof. The present invention also relates to computer readable media encoded with sets of the three-dimensional coordinates of the *E. coli* MurG protein, the α-carbon backbone of the MurG protein, the α-carbon backbone and the conserved amino acid residue sidechains of the MurG protein, the donor nucleotide binding site, the acceptor binding site, and the membfane association site. The present invention relates to methods of crystallizing MurG proteins.

The present invention relates to models of three-dimensional structures of UDP-glycosyltransferases and, in particular, MurG proteins, based on the three-dimensional structure of crystals of the *Escherichia coli* MurG. The present invention also relates to models of the three-dimensional structures of the α-carbon backbone of UDP-glycosyltransferases and MurG proteins. The present invention further relates to

models of the three-dimensional structure of the α-carbon backbone and conserved amino acid residue sidechains of UDP-glycosyltransferases, in particular, MurG proteins. The present invention further relates to models of the three-dimensional structures of donor nucleotide binding sites, acceptor binding sites, and membrane association sites of UDP-glycosyltransferases, in particular, MurG proteins. The present invention also relates to methods of drug design using models of this invention. The present invention further relates to compounds identified using models of the present invention that bind, inhibit or stimulate UDP-glycosyltransferases or MurG proteins. The present invention relates to compositions comprising compounds identified using the models of this invention for therapeutic or diagnositic uses. Also, the present invention relates to methods of making models of the present invention.

BACKGROUND OF THE INVENTION

The increasing frequency of resistance to existing antibiotics represents a serious public health threat. Structural and mechanistic information on essential bacterial enzymes could lead to the development of antibiotics that are active against resistant microorganisms. Both gram positive and gram negative bacterial cells are surrounded by a cross-linked carbohydrate polymer, peptidoglycan, which protects them from rupturing under high osmotic pressures. Many of the best antibiotics function by inhibiting peptidoglycan synthesis, which ultimately causes cell lysis. In recent years, intense effort has been focused on determining the structures of the enzymes that synthesize peptidoglycan. Structures of several of the early enzymes in the biosynthetic pathway have been reported (Benson *et al.,* 1995; Bertrand *et al.,* 1997; Fan *et al.,* 1994; Skarzynski *et al.,* 1996); however, the later enzymes have proven more difficult to study because both they and their substrates are membrane-associated.

MurG is the last enzyme involved in the intracellular phase of peptidoglycan synthesis (Bugg & Walsh, 1993). It catalyzes the transfer of N-acetyl glucosamine (NAG) from UDP to the C4 hydroxyl of a lipid-linked N-acetylmuramoyl pentapeptide (NAM) to form a β-linked NAG-NAM disaccharide that is transported across the cell membrane where it is polymerized and cross-linked (Fig. 1). In bacterial cells MurG associates with the cytoplasmic surface of the membrane (Bupp & van Heijenoort, 1993). However, we have found that *E. coli* MurG can be solubilized at high concentrations in active form (Ha et al., 1999).

The elucidation of the protein structure of a MurG protein is of importance in the identification and formulation of anti-bacterial agents. Until the discovery of the present invention, the structure and resulting mechanism by which MurG functions was not known. Thus, despite the important role of MurG in peptidoglycan synthesis, development of useful agents for treatment or diagnosis of disease was hindered by lack of structural information of the protein.

In order to obtain structural information on a MurG protein, it is important to have purified, active enzyme. The demonstration of activity requires a suitable assay, which in turn requires access to the natural substrates or analogues thereof. The study of MurG was hampered by difficulties obtaining and handling the lipid-linked NAM substrate (commonly known as Lipid I). This problem was overcome by Walker and coworkers, who developed a synthetic route to a set of substrate analogues of Lipid I that were shown to function as glycosyl acceptors in a glycosyl transfer reaction catalyzed by MurG. Some of these substrate analogues are freely water soluble, making it possible to monitor the activity of purified *E. coli* MurG in buffer in the absence of natural or artificial membranes or detergents.

The linear nucleic acid and amino acid sequences of *E. coli* MurG were reported in 1992. Subsequently, the nucleic acid and amino acid sequence of *B. subtilus* MurG was reported. Since then, many bacterial genomes have been sequenced and the information has been deposited in databases. Information based only on linear sequences, however, cannot accurately predict the three-dimensional structure of the protein and its functional domains.

Therefore, there is a need in the art to elucidate the three-dimensional structure of a MurG protein. One three-dimensional structure of a MurG protein can be used to construct models of other MurG proteins and to facilitate the structure determination of crystalline forms of other MurG proteins. Structures and models of MurG proteins can also be used to design proteins containing only the donor binding site or the acceptor binding site. These proteins can be used in assays, including NMR-based assays, to identify -- or characterize the mode of binding of -- ligands that bind in or near the vicinity of the substrates. These ligands or compounds can then be used as leads for the design of inhibitors that have therapeutic activity. Structures and models of MurG proteins can also be used in computer-based drug design.

SUMMARY OF THE INVENTION

The present invention relates to crystalline *Escherichia* coli MurG protein. Obtaining such crystals is an unexpected result. It is well known in the protein crystallographic art that obtaining crystals of quality sufficient for determining the structure of a protein is unpredictable. In particular, obtaining crystals of quality sufficient for determining the three-dimensional (3-D) structure of MurG has not been achievable until the crystallization of MurG as disclosed in the present application. As such, determination of the three-dimensional structure of MurG has not been possible until the discovery of the present invention. Additionally, until the discovery of the present invention, derivation of the three-dimensional structure and models of other MurG proteins has not been possible. The present inventors are also the first to define the three-dimensional structure and provide three-dimensional models for drug design for MurG proteins.

Accordingly, one object of the present invention is to provide crystals of sufficient quality to obtain a determination of the three-dimensional atomic coordinates and structures of MurG to high resolution, preferably to the resolution of less than 2.0 angstroms (A). The present invention also provides methods for producing crystalline MurG protein.

The value of the crystals of *E. coli* MurG protein extends beyond merely being able to obtain such crystals. The knowledge obtained concerning the MurG crystal structure, for example, has been used by the present inventors to define the heretofore unknown tertiary structure of the MurG protein and to identify the location of the glycosyl donor and glycosyl acceptor binding domains, as well as the location of the amino acid residues that are invariant in all MurG proteins. This information can be used to design inhibitors of MurG that have therapeutic utility. The atomic coordinates of *E. coli* MurG also are used to model the heretofore unknown tertiary structures of other MurG proteins having substantially related linear amino acid sequences, such as for MurG proteins from other microorganisms. It is anticipated that homology models can be constructed even from amino acid sequences with relatively low homology because the present inventors have identified the location of the invariant amino acid residues in MurG. The relative spatial orientations of such residues is expected to be conserved in all MurG proteins.

Comparison of nucleic acid and amino acid sequences of MurG proteins indicates that the linear amino acid sequences can vary significantly. Homology between MurG proteins from different microorganisms varies from less than 30% to greater than 90%, reflecting the evolutionary relationship between the organisms. The low homology between distantly related MurG homologues is not believed to reflect significantly different folded structures. It is well known that many amino acid sequences are capable of adopting the same general fold. *E. coli* MurG contains an alpha/beta folding pattern, one of the most common folds known in proteins. It is likely that all MurG homologues contain a similar alphalbeta fold despite the differences in the linear amino acid sequences. What gives these proteins their identity is not the general fold, but the specific details - i.e., the presentation of certain amino acids on the folded structure. The present inventors have identified the location in *E. coli* MurG of a set of residues that are invariant in all MurG homologues. It is to be expected that these residues would adopt a similar spatial location with respect to the folded structure in all MurG homologues. Therefore, these invariant residues, which have been selected by evolution as the critical residues for the binding and catalytic function of the protein, provide essential information on the location of the active site and on critical contacts to the substrates/products. They also serve as constraints that make it possible to, predict the three-dimensional structures even of distantly related MurG homologues. Thus, knowledge of the three-dimensional structure of the *E. coli* MurG protein has provided a starting point for investigation into the structure of all MurG proteins.

Accordingly, a object of the present invention is to provide information regarding the atomic coordinates and three-dimensional structures of (1) the MurG protein, (2) the α-carbon backbone of the MurG protein, (3) the α-carbon backbone and conserved amino acid residues of the MurG protein, (4) the donor nucleotide binding site, (5) the acceptor binding site, and (6) the membrane association site MurG proteins.

It is also an object of this invention to solve the three-dimensional structure of UDP-glycosyltransferases, in particular target NTURG proteins, and to determine their structure and/or atomic coordinates. Further, it is an object of this invention to use the structure or atomic coordinates of the *E. coli* MurG crystal to solve the structure of different MurG protein crystals, or a crystal of a mutant protein, homolog or co-complex of MurG.

The present invention relates to models of three-dimensional structures of UDP-glycosyltransferases, in particular MurG proteins, based on the atomic coordinates of crystalline *E. coli* MurG protein.

It is a further object of this invention to provide, UDP-glycosyltransferase enzyme mutants characterized by one or more different properties as compared with wild-type MurG. These properties include altered surface charge, increased stability to subunit dissociation, altered substrate specificity or higher specific activity. MurG mutants are useful to identify those amino acids that are most important for the enzymatic activity of MurG. This information, in turn, allows the design of improved inhibitors of MurG as compared with peptidic MurG inhibitors.

Another object of the present invention is to provide computer readable mediums encoded with a set of three-dimensional coordinates of the *E. coli* MurG protein, the α-carbon backbone of the MurG protein, the α-carbon backbone and conserved amino acid residues of the MurG protein, and the nucleotide donor binding site, the acceptor binding site, the membrane association site of the MurG protein.

Another embodiment of the present invention provides three-dimensional and two-dimensional computer images of the three-dimensional structure of MurG protein, the α-carbon backbone of the MurG protein, the α-carbon backbone and conserved amino acid residues of the MurG protein, and the nucleotide donor binding site, the acceptor binding site, the membrane association site of the MurG protein.

The knowledge of the three-dimensional structure of MurG also provides a means for designing proteins that have altered beneficial functions by analyzing the structure and interactions between individual amino acids of the protein. For example, the present inventors have shown that *E. coli* MurG consists of two domains separated by a cleft.

Noncovalent interactions between the two domains are not extensive. The present inventors have shown that the domains fold independently and can, therefore, be expressed independently either alone or as part of a recombinant protein containing the acceptor binding site from one MurG homologue and the donor binding site from another MurG homologue. It would be expected that the domains of other MurG proteins could also be expressed independently, either alone or as chimaeras with other

MurG domains. Independently expressed domains of the protein are useful for discovering ligands that bind to the individual domains.

The knowledge of the three-dimensional structure of *E. coli* MurG protein and models of other MurG proteins also provides a means for designing and producing compounds that regulate, inhibit or antagonize functions of the MurG protein (i.e., structure based drug design). For example, chemical compounds can be designed to block binding of UDP-GlcNAc to a MurG protein using various computer programs and models.

It is also an object of this invention to use the structure coordinates and atomic details of MurG, or its mutants or homologues or co-complexes, to design, evaluate computationally, synthesize and use inhibitors of MurG that avoid the undesirable physical and pharmacologic properties of peptidic MurG inhibitors.

Another embodiment of the present invention is a composition comprising MurG protein in a crystalline form.

Yet another embodiment of the present invention is a method for producing crystals of MurG, comprising combining MurG protein in a suitable buffer with a suitable amount of a reservoir buffer containing a detergent, and inducing crystal formation to produce said MurG crystals.

BRIEF DESCRIPTION OF THE DRAWINGS

Fig. 1. Pathway for peptidoglycan biosynthesis.

Fig. 2. Overall architecture of MurG. A. Stereo view of the MurG structure. The N domain is shown in purple; the C domain is shown in green. The figure was generated with the programs MOLSCRIPT (Klaulis, 1991) and RASTER31) (Merrit & Murphy, 1994). B. Topology diagram of MurG.

Fig. 3. Identification of critical residues in MurG and related glycosyltransferases. A. Sequence alignment of *E. coli* MurG with homologs from seven other bacterial strains, deliberately chosen to represent a disparate group of organisms. The secondary structure of *E. coli* MurG is shown above the sequences. Gaps mapping to the loop regions of *E. coli* MurG suggest that some sequences include other structural elements. Residues highlighted in blue are invariant among the eighteen MurG sequences available. Residues highlighted in yellow are identical in 85% of the eighteen homologs, while in the remaining 15%, only closely related amino

acid substitutions are found. Highly conserved residues that do not meet the stringent criteria established for highlighting are shown in the consensus sequence. A consensus motif for UDP-glucuronosyltransferases is also shown. Numbering is with respect to the overexpressed *E. coli* MurG construct, which contains an additional N-terininal methionine. B. Mapping of the G loops and other highlighted residues from Fig. 3a in red on the MurG structure. Side chains for highly conserved residues are also shown. C. Model for the proposed UDP-binding subdomain found in many UDP-glycosyltransferases based on the *E. coli* MurG structure. Conserved residues in UDP-glucuronosyltransferases are highlighted in red. Side chains are shown for residues that are located near the cleft and may be involved in substrate binding. The glutamate residue is proposed to interact with the ribose sugar. The dotted loop varies in length within the MurG family and in other UDP-sugar transferases, but the N and Q on the following helix are invariant. Note that the UDPglucuronosyltransferases contain a conserved D preceding the Q, which is not shown on this model.

Fig 4. Structural analysis of the substrate binding pockets in MurG. A. Structural comparison between the C-terminal domain of phage T4 β-glucosyltransferase (left) and the C-terminal domain of *E. coli* MurG (right). The aligned six β-strands are magenta, the aligned α-helices are orange, and the other structural elements are blue. In β-glucosyltransferase, key residues involved in UDP binding are highlighted in yellow. The analogous residues in MurG are also highlighted in yellow. B. A close-up view of the proposed donor binding pocket in the MurG C domain with the docked UDP-GlcNAc. Conserved residues in MurG are colored magenta. The carbonyl oxygen of residue 1245 is shown in red, and its backbone nitrogen is shown in blue. C. The surface of *E. coli* MurG. The G loops and other conserved residues in MurG are colored magenta. The proposed membrane binding interface is also highlighted with hydrophobic residues in yellow and positively charged residues in blue.

DEFINITIONS

It is to be noted that the term "a" or "an" entity refers to one or more of that entity; for example, a compound refers to one or more compounds or at least one compound. As such, the terms "a" (or "an"), "one or more", and "at least one" can be used interchangeably herein.

It is also to be noted that the terms "comprising", "including" and "having" can be used interchangeably. Furthermore, a compound "selected from the group consisting of" refers to one or more of the compounds in the list that follows, including mixtures (i.e., combinations) of two or more of the compounds.

According to the present invention, an isolated, or pure, protein, is a protein that has been removed form its natural milieu. As such, "isolated" and "biologically pure" do not necessarily reflect the extent to which the protein has been purified. An isolated protein of the present invention can be obtained from its natural source, can be produced using recombinant DNA technology or can be produced by chemical synthesis.

It is also to be noted that the terms "tertiary" and "three-dimensional" can be used interchangeably.

It is also to be noted that reference to a "MurG protein" can also be recited as "MurG" and such terms can be used to refer to the complete MurG protein, a portion of the MurG protein, such as a polypeptide.

The following terms are also used herein:

The term "naturally occurring amino acids" means the L-isomers of the naturally occurring amino acids. The naturally occurring amino acids are glycine, alanine, valine, leucine, isoleucine, serine, methionine, threonine, phenylalanine, tyrosine, tryptophan, cysteine, proline, histidine, aspartic acid, asparagine, glutamic acid, glutamine, gamma-carboxyglutamic acid, arginine, ornithine and lysine. Unless specifically indicated, all amino acids referred to in this application are in the L-form.

The terin "unnatural amino acids" means amino acids that are not naturally found in proteins. Examples of unnatural amino acids used herein, include racemic mixtures of selenocysteine and selenomethionine. In addition, unnatural amino acids include the D or L forms of nor-leucine, para-nitrophenylalanine, homophenylalanine, parafluorophenylalanine, 3-amino-p2-benzylpropionic acid, homoarginine, and D-phenylalanine.

The term "positively charged amino acid" includes any naturally occurring or unnatural amino acid having a positively charged side chain under normal physiological conditions. Examples of positively charged naturally occurring amino acids are arginine, lysine and histidine.

The term "negatively charged amino acid" includes any naturally occurring or unnatural amino acid having a negatively charged side chain under normal physiological conditions. Examples of negatively charged naturally occurring amino acids are aspartic acid and glutamic acid.

The term "hydrophobic amino acid" means any amino acid having an uncharged, nonpolar side chain that is relatively insoluble in water. Examples of naturally occurring hydrophobic amino acids are alanine, leucine, isoleucine, valine, proline, phenylalanine, tryptophan and methionine.

The term "hydrophilic amino acid" means any amino acid having an uncharged, polar side chain that is relatively soluble in water. Examples of naturally occurring hydrophilic amino acids are serine, threonine, tyrosine, asparagine, glutamine, and cysteine.

The term "MurG" refers to a UDP-glycosyltransferase that has a two domain strucuture, where each domain contains a set of invariant residues as shown in Fig. 3a, including any mutant, homologue or co-complex or any similar enzyme that catalyzes the transfer of N-acetylglucosamine (GlcNAc) from UDP to the C4 hydroxyl of the lipidlinked MurNAc pentapeptide.

The term "mutant" refers to a MurG polypeptide, i.e., a polypeptide displaying the biological activity of a wild-type MurG, characterized by the replacement of at least one amino acid from the wild-type, *E. coli* MurG sequence according to Ikeda, et al., Nucleic Acids Res. 1990, and Mengin-LeCreuix et al., Nucleic Acids Res. 1990. Such a mutant may be prepared, for example, by expression of MurG cDNA previously altered in its coding sequence by PCR-based mutagenesis method.

MurG mutants may also be generated by site-specific incorporation of unnatural amino acids into MurG proteins using the general biosynthetic method of Noren, C. J., et al., Science, 244, pp.182-188 (1989). In this method, the codon encoding the amino acid of interest in wild-type MurG is replaced by a "blank" nonsense codon, TAG, using oligonucleotide-directed mutagenesis (described in detail, infra). A suppressor tRNA directed against this codon is then chemically aminoacylated in vitro with the desired unnatural amino acid. The aminoacylated tRNA is then added to an in vitro translation system to yield a mutant MurG enzyme with the site-specific incorporated unnatural amino acid.

Selenocysteine or selenomethionine may be incorporated into wild-type or mutant MurG by expression of MurG-encoding cDNAs in auxotrophic *E. coli* strains. Hendrickson, W. A. et al., EMBO J., 9(5), pp. 1665-1672 (1990). In this method, the wild-type or mutagenized MurG CDNA may be expressed in a host organism on a growth medium depleted of either natural cysteine or methionine (or both) but enriched in selenocysteine or selenomethionine (or both).

The term "altered surface charge" means a change in one or more of the charge units of a mutant polypeptide, at physiological pH, as compared to wild-type MurG. This is preferably achieved by mutation of at least one amino acid of wild-type MurG to an amino acid comprising a side chain with a different charge at physiological pH than the original wild-type side chain.

The change in surface charge is determined by measuring the isoelectric point (pI) of the polypeptide molecule containing the substituted amino acid and comparing it to the isoelectric point of the wild-type MurG molecule.

The term "altered substrate specificity" refers to a change in the ability of a mutant MurG to cleave a substrate as compared to wild-type MurG.

The "kinetic form" of MurG refers to the condition of the enzyme in its free or unbound form or bound to a chemical entity at either its active site or accessory binding site.

A "competitive" inhibitor is one that inhibits MurG activity by binding to the same kinetic form of MurG as its substrate binds—thus directly competing with the substrate for the active site of MurG. Competitive inhibition can be reversed completely by increasing the substrate concentration.

An "uncompetitive" inhibitor is one that inhibits MurG by binding to a different kinetic form of the enzyme than does the substrate. Such inhibitors bind to MurG already bound with the substrate and not to the free enzyme. Uncompetitive inhibition cannot be reversed completely by increasing the substrate concentration.

A "non-competitive" inhibitor is one that can bind to either the free or substrate bound form of MurG.

Those of skill in the art may identify inhibitors as competitive, uncompetitive or non-competitive, by computer fitting enzyme kinetic data using standard equations according to Segel, I. H., Enzvme Kinetics, J. Wiley & Sons, (1975). It should also be

understood that uncompetitive or non-competitive inhibitors apcording to this invention may bind to the accessory binding site.

The term "homolog" means a protein having at least 25% amino acid sequence identity with MurG or any functional part of MurG, and including certain invariant amino acid residues corresponding to G14, G15, G18, H19, G104, H124, E125, G190, G191, S192, G194, A195, R261, G263, A264, E269, P281, Q289, N292 and A293 (as numbered in the E.coli MurG sequence set forth in Fig. 3a) and also including three glycine rich loops. A homolog may contain some or all of the invariant residues.

The term "co-complex" means MurG or a mutant or homologue of MurG in covalent or non-covalent association with a chemical entity or compound.

The term "associating with" refers to a condition of proximity between a chemical entity or compound, or portions thereof, and a MurG molecule or portions thereof. The association may be non-covalent--wherein the juxtaposition is energetically favored by hydrogen bonding or van der Waals or electrostatic interactions--or it may be covalent.

The term ".beta.-sheet" refers to the conformation of a polypeptide chain stretched into an extended zig-zig conformation. Portions of polypeptide chains that run "parallel" all run in the same direction. Polypeptide chains that are "antiparallel" run in the opposite direction from the parallel chains.

The terms "atomic coordinates" or "structure coordinates" refer to mathematical coordinates derived from mathematical equations related to the patterns obtained on diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) of a MurG molecule in crystal form. The diffraction data are used to calculate an electron density map of the repeating unit of the crystal. The electron density maps are used to establish the positions of the individual atoms within the unit cell of the crystal.

The term "heavy atom derivatization" refers to the method of producing a chemically modified form of a crystal of MurG. In practice, a MurG crystal is soaked in a solution containing heavy metal atom salts, or organometallic compounds, e.g., lead chloride, gold thiomalate, thimerosal, uranyl acetate or mercuric chloride, which can diffuse through the crystal and bind to the surface of the protein. The location(s) of the bound heavy metal atom(s) can be deetermined by X-ray diffraction analysis of the soaked crystal. This information, in turn, is used to generate the phase information used

to construct three-dimensional structure of the enzyme. Blundel, T. L. and N. L. Johnson, Protein Crystallography, Academic Press (1976).

Those of skill in the art understand that a set of structure coordinates determined by X-ray crystallography is not without standard error. For the purpose of this invention, any set of structure coordinates for MurG or MurG homologues or MurG mutants that have a root mean square deviation of protein backbone atoms (N, C.alpha., C and 0) of less than 0.75 Å when superimposed--using backbone atoms--on the structure coordinates listed in Table 1, Table 2 or Table 3 shall be considered identical.

The term "unit cell" refers to a basic parallelepiped shaped block. The entire volume of a crystal may be constructed by regular assembly of such blocks. Each unit cell comprises a complete representation of the unit of pattern, the repetition of which builds up the crystal.

The term "space group" refers to the arrangement of symmetry elements of a crystal.

The term "molecular replacement" refers to a method that involves generating a preliminary model of a MurG crystal whose structure coordinates are unknown, by orienting and positioning a molecule whose structure coordinates are known (e.g., MurG coordinates from Table 1, 2, or 3) within the unit cell of the unknown crystal so as best to account for the observed diffraction pattern of the unknown crystal. Phases can then be calculated from this model and combined with the observed amplitudes to give an approximate Fourier synthesis of the structure whose coordinates are unknown. This, in tum, can be subject to any of the several forms of refinement to provide a final, accurate structure of the unknown crystal. Lattman, K., "Use of the Rotation and Translation Functions", in Methods in Enzymology, 115, pp. 55-77 (1985); M. G. Rossmann, ed., "The Molecular Replacement Method", Int. Sci. Rev. Ser., No. 13, Gordon & Breach, New York, (1972). Using the structure coordinates of MurG provided by this invention, molecular replacement may be used to determine the structure coordinates of a crystalline mutant or homologue of MurG or of a different crystal form of MurG.

DETAILED DESCRIPTION OF THE INVENTION

The present invention relates to the discovery of the three-dimensional structure of the crystalline form of the *E. coli* MurG protein, models of such three-dimensional

structures, a method of structure based drug design using such structures, methods to identify ligands or compounds that interact or bind with such structures, the compounds identified by such methods, and the use of such compounds in therapeutic compositions.

More particularly, the present invention relates to novel crystals of *E. coli* MurG protein, methods of production of such crystals, three-dimensional coordinates of MurG protein, MurG structures and models derived from the *E. coli* MurG structure, and uses of such structures and models to derive other MurG structures and in ligand discovery and drug design strategies.

The present invention also relates to three-dimensional structures and coordinates of the donor nucleotide binding site, the acceptor binding site, and the membrane association site of the MurG protein, structures and models of the binding sites, and uses of such structures and models to derive the binding sites of other MurG proteins and in drug design strategies.

Solely for ease of explanation, the description of the invention is divided into the following sections: (1) crystals of MurG protein; (2) methods of crystallization; (3) three-dimensional crystal coordinates and structure of *E. coli* MurG; (4) three-dimensional coordinates and structure of the donor nucleotide binding site of MurG; (5) coordinates and structure of the acceptor binding site of MurG; (5) three-dimensional coordinates and structure of the membrane association site; (6) two-dimensional and three-dimensional images of the protein, α-carbon backbone, α-carbon backbone with conserved amino acid residues, and binding sites; and (7) computer readable mediums comprising the three-dimensional coordinates of the MurG protein, α-carbon backbone, α-carbon backbone with conserved amino acid residues, and binding sites; (8) images of structures of MurG protiensand binding sites; (9) models of MurG proteins and binding sites thereof and methods of using the structure of MurG to determine the structures of other MurG proteins and binding sites; (10) structure based drug design using models of MurG protein and binding site structures; (11) compounds derived from structure based drug design; and (12) therapeutic compositions using drugs designed from structure based drug design.

CRYSTALS

One embodiment of the present invention includes a pomposition comprising a MurG protein in a crystalline form (i.e., MurG crystals). As used herein, the terms (crystalline MurG" and "MurG crystal" both refer to crystallized MurG protein and are intended to be used interchangeably. More particularly, an embodiment of the present invention includes a composition comprising an *E. coli* MurG protein in a crystalline form. Preferably, a crystalline MurG is produced using the crystal formation method described herein, in particular according to the method disclosed in Example 1. A MurG crystal of the present invention comprises any crystal structure and preferably precipitates as a triclinic crystal. Preferably, a composition of the present invention includes MurG crystal molecules arranged in a crystalline manner in a P1 space group with two molecules per assymmetric unit so as to form a unit cell of dimensions a=60.613 Å, b=66.356 Å, c=67.902 Å, α=64.294, β=83.520, γ=65.448. A preferred crystal of the present invention provides X-ray diffraction data for determination of atomic coordinates to a resolution of about 3.0 Å, preferably to about 2.4 Å, and more preferably to about 1.8 Å.

Another embodiment of the present invention includes crystalline MurG protein co-crystallized with a donor nucleotide or substrate or substrate analog. Preferably, a donor nucleotide is UDP or UDP-GlcNAc (UDP-N-acetylglucosamine) or an analog thereof. The substrate or substrate analog is preferably Lipid I or Lipid II or analogs of Lipid I or Lipid II. More specifically, Lipid I and II analogs are as described in PCT/US99/02187, published as W099/38958 and US Provisional Application Nos. 60/122,966 filed March 3, 1999 and 60/137,696 filed June 4, 1999, and International Application No. PCT/US00/05554 entitled "Bacterial transglycosylases: Assays for monitoring the activity using Lipid II substrate analogs and methods for discovering antibiotics," all incorporated herein by reference in their entirety.

Included in the present invention, a variety of MurG proteins from numerous organisms can be used to prepare MurG crystals, including but not limited to, microorganisms such as bacteria, higher-order bacteria, thermal stable bacteria, spirochetes, small pathogenic organisms, fungi, protozoa, cyanobacteria, and trypanosomes. More particularly, bacteria such as but not limited to, *Escherichia coli, Bacillus subtilis, Aquefe-x aeolicus, Borrelia burgdorferi, Chlamydia pneumoniae, Chlamydia trachomatis, Enterococcus jaecais, Enterococcus hirae, Haemophilus*

influenzae, Helicobacter pylori J99, Helicobacter pylori, Mjrobacterium tuberculosis, Porphyromonas gingivalis, Rickettsia prowazekii, Streptomyces coelicolor, Streptomyces collinus, Streptococcus pneumoniae, Synechocystis sp. (strain PCC6803), *Thermotoga maritime,* and *Treponemapallidum.*

In another embodiment of the present invention, the MurG proteins or fragments thereof, mutants or homologs are expressed in, for example, an *E. coli* host cell for use expressing sufficient quantities of sufficiently purified protein to form crystals. The present inventors have demonstrated that it is possible to express *Enterococcus. jaecalis* MurG in *E. coli* cells - so the MurG proteins from many organisms can be cloned into expression vectors suitable for expression in *E. coli* cells. This would facilitate obtaining sufficient quanitites of isolated or purified MurG proteins. The expression of E. *jaecalis* MurG protein in *E. coli* host cells is performed, for example, by expressing the E. *jaecalis* MurG gene cloned into a pET21b expression vector and transformed into an *E. coli* host cell. The MurG protein is over-expressed with a C-terminal his tag (LEHHHHHH) which allows the protein to be purified using a His-tag affinity column. The protein is then crystallized and the atomic coordinates are determined using X-ray diffraction and methods known to those skilled in the art.

It is another embodiment of the present invention to provide for the construction and expression of chimaeric MurG proteins to enable the crystallization and determination of the three-dimensional coordinates of such chimeras. For example, if there are problems obtaining or crystallizing MurGs from other organisms, the present invention provides information that makes it possible to make chimaeric proteins containing the donor or acceptor binding site from *E. coli* MurG and the corresponding acceptor or donor binding site from another organism. Chimaeric proteins could be easier to express, handle, or crystallize. For example, we have found that E. faecalis MurG is more difficult to solubilize that *E. coli* MurG (requiring more detergent). It is believed that the problems are related to the acceptor binding domain having a stronger affinity for the bacterial membranes. To overcome this problem, one can attach the donor binding domain of *E. faecalis* to the *E. coli* acceptor binding site and determine structure to see details of *E. faecalis* donor binding domain.

According to the present invention, crystalline MurG can be used to determine the ability of a chemical compound to bind to a MurG protein in a manner predicted by

a structure based drug design method of the present invention. Preferably, a MurG crystal is soaked in a solution containing a chemical compound of the present invention. Binding of the chemical compound to the crystal is then determined by methods standard in the art. Thereby, the co-crystal of MurG and a compound of interest is determined.

METHODS OF CRYSTALLIZATION

The present invention includes a method for producing crystals of MurG proteins, comprising: combining MurG protein with a reservoir solution and inducing crystal formation to produce MurG crystals. Another embodiment of the present invention, a method for producing crystals of MurG protein comprises combining MurG protein with UDP-GlcNAc in a 1:3 ratio and with a reservoir solution and inducing crystal formation to produce MurG crystals.

Preferably, crystals of MurG are formed using a solution containing a range of MurG protein from about 1 mg/ml to about 20 mg/ml, more preferably above 5 mg/ml, limited only by the solubility of the protein, which may vary depending on the specific amino acid sequence.

A reservoir solution contains the buffer, the precipitant, and additives if necessary. A suitable reservoir buffer of the present invention comprises NaMES (2-[N-morpho]inolethanesulfonic acid, sodium salt) buffer, NaHEPES (N-[2-hydroxyethyl]piperazine-N'-[2-ethanesulfonic acid, sodium salt) buffer, Tris (tris[hydroxymethyl]aminomethane) buffer, and any buffer which has the PKa between 5.5 and 8.0. A suitable NaMES buffer solution has a pH range from about 5.6-6.5. Most preferably, the NaMES buffer has a pH of about 6.5. The precipitant comprises ammonium sulfate, saturated sodium and potassium tartrate and polyethylene glycol. A suitable concentration of ammonium sulfate can range from 0.8 M to 1.5 M. Most preferably, the ammonium sulfate concentration is about 0.96 M. A suitable additive comprises detergents like Triton X-100 and n-octyl-beta-glucoside. The concentration of Triton X-100 can range from 0.1% to 1%. Most preferably, the concentration of Triton X-100 is 0.4%.

In a preferred embodiment, MurG crystals are produced by a method comprising concentrating MurG protein in a buffer solution, mixing the protein concentrate with

UDP-GlcNAc in a 1:3 molar ratio, mixing equal volumes of protein solution with a reservoir solution, and inducing crystal formation to produce MurG crystals.

In a particular embodiment of the invention, MurG crystals are produced by a method comprising concentrating MurG protein to 10 mg/ml in a buffer of 20 mM Tris-HCl, pH 7.9/150mM NaCl and 50 mM EDTA; mixing the protein concentrate with UDP-GlcNAc in a 1:3 molar ratio; mixing equal volumes of protein solution with a reservoir solution comprising (0.1 M NaMES, pH 6.5, 0.96 M $(NH_4),SO_4$, 0.4% TRITON® X-100, and 10 mM dithiolthreitol (DTT)), and inducing crystal formation using hanging drop vapor-diffusion. This preferred method is described in greater detail in Example 1.

Supersaturated solutions of MurG protein can be induced to crystallize by several methods including, but not limited to, vapor diffusion, liquid diffusion, batch crystallization, constant temperature and temperature induction or a combination thereof. Preferably, supersaturated solutions of MurG protein are induced to crystallize by vapor diffusion (i.e., hanging drop method). In a vapor diffusion method, a MurG protein solution is combined with a reservoir solution of the present invention that will cause the MurG protein solution to become supersaturated and form MurG crystals at a constant temperature. Vapor diffusion is preferably performed under a controlled temperature in the range of from about 15° C to about 30° C, more preferably from about 20° C to about 25° C, and most preferably at a constant temperature of about 22° C.

In another preferred embodiment, the present invention includes a method to produce crystals of MurG protein comprising the steps of: (a) preparing an about 10 mg/ml solution of MurG protein in a Tris-HCl buffer, (mixing UDP-GlcNAc with the Mur-G protein solution in a 3:1 molar ratio, (c) dropping 2 µl droplet of this protein sample onto a coverslip, (d) adding an equal volume of reservoir solution to this droplet and inverting this over a well containing about 1 ml of the reservoir solution; and (e) incubating until crystals of MurG form.

Any isolated MurG protein can be used with the present method. An isolated MurG protein can be isolated from its natural milieu or produced using recombinant DNA technology (e.g., polymerase chain reaction (PCR) amplification, cloning) or chemical synthesis. To produce recombinant MurG protein, a nucleic acid molecule

encoding a MurG protein can be inserted into any vector capable of expressing the nucleic acid in a host clell. Suitable and preferred nucleic acid molecules to include in recombinant vectors of the present invention are as disclosed herein. Such suitable and preferred nucleic acid molecules include numerous MurG encoding genes that have been isolated to date, and that will be isolated in the future. A preferred nucleic acid molecule of the present invention encodes a homologue of MurG. Homologues of MurG can be recognized by the presence of certain conserved amino acid residues or sequences.

A sequence alignment for six MurG sequences is shown in Fig. 3A. Highlighted residues include those that are invariant or almost invariant across all MurG proteins. A nucleic acid molecule of the present invention can encode any portion of a MurG protein, preferably a full-length MurG protein or either of the two domains. A more preferred nucleic acid molecule to include in a recombinant vector, and particularly in a recombinant molecule, includes a nucleic acid molecule encoding a protein having the amino acid sequence represented by amino acid sequences of MurG proteins as deposited in the NCBI database and are identified with Accession Nos. CAB51993, A71316, E70579, C71699, F70195, A43727, JC1275, BVECMG, CEECAM, O83535, Q9ZK59, CAB85280, AAF39020, BAA18775, AAD26629, CAB73295, P37585, Q9ZHA9, Q9ZHDC0, Q9ZBA5, Q9X4H4, Q9WY74, P74657, O06224, Q9Z702, O84766, O69552, O67238, O51708, O25770, O07670, O07109, P45065, CAB66324, AAC68356, AAF06830, P18579, P17443, P17952, P16457, P07862, AAE23178, AAD53936, CAA18668, CAA38869, CAA38868, CAA38867, CAA38866, AAD08196, BAA01453, BAA01455, BAA01454, AAD19042, CAA45558, CAA74235, AAD10537, AAD06652, AAC95450, CAA14869, AAC73201, AAC65509, AAC67113, AAC45636, CAB08640, AAC22793, AAC07193, BAA24357, CAB13395, BAA01355, AAB35538, 1904153C, 1808265B, 1808265A, CAA36866, CAA36869, CAA36868, CAA36867, CAA36776, and AAA99436. Further, examples of nucleic acid molecules encoding MurG proteins have been deposited in NCBI, Genbank, and have Accession Nos. AL162758, AE002281, D90917, AF110367, AL139077, AJ242646, AE000520, AE000511, L42023, U00096, NC-000922, AE000783, AE000657, AE001348, AF099188, AR048673, AR048672, AF179611, AL022602, AL109663, X55034, AE000621,

D10602, AE001670, X64259, Y13922, U10879, AE001535, AF068902, AJ235271, AE000118, AE001227, AE001176, U94707, Z95388, U32793, AE000727, D84504, Z99111, D10483, X52644, X52540, and L24773. These sequences are known and are publicly available. Further, as additional genomes and genes are sequenced, more MurG encoding nucleotide sequences will become available, and can be used in the present invention.

In specific embodiments of the invention, the protein sequence of *E. coli* MurG was reported in 1990 (Ikeda et al. Nucleic Acids Res. 1990, 19:4014; and Mengin-Lecreuix, D. et al., Nucleic Acids Res. 1990, 18:2810.). *E. coli* genomic DNA can be purified from *E. coli* or purchased from ATCC, or the gene for *E. coli* MurG is cloned into a plasmid can be obtained from numerous sources. Primers were designed to the portions of the gene corresponding to the N and C termini of the protein. The primers also encoded restriction enzyme sites outside the protein coding region. The gene sequence was amplified; the corresponding double stranded nucleic acid molecule was cut with appropriate restriction enzymes for cloning into a commercially available expression vector (pET expression vectors available from Novagen provide for numerous variations of MurG protein - wild-type or fusion proteins or proteins with affinity tags at N or C terminus. We have worked with several constructs but found that MurG with a His-tag at C-terminus crystallized best; the protein sequence contained an extra methionine at N-terminus and eight extra residues at C terminus, six of which were histidines. The vector used was pET21b. (as described in Ha et al. J. Am. Chem. Soc. 121, (1999) 8415-8426 hereby incorporated by reference in its entirety).

A recombinant vector of the present invention can be either RNA (probably not) or DNA, and typically includes, but is not limited to, a virus or plasmid. Any recombinant vector and host cell that provides for expression of a MurG protein encoding mucleic acid sequence can be used in the present invention to express MurG protein for crystallization. Preferred vectors are engineered for high level expression in *E. coli* such as, but not limited to, pET vectors. We have found that over-expression of MurG from either *E. coli* or *E. faecalis* in *E. coli* cells is not toxic and, thus, this approach will work for other MurG proteins.

As used herein, an expression vector is a DNA vector that is capable of transforming a host cell and of affecting expression of a specified nucleic acid

molecule. Expression vectors of the present invention include any vectors that function (i.e., direct gene expression) in recombinant cells of the present invention, including bacterial, fungal, and other microorganisms cells. Preferred expression vectors of the present invention direct expression in bacterial cells from a plasmid. A preferred recombinant molecule of the present invention comprises pET21b with *E. coli* MurG gene cloned into the Nde 1 and Xho 1 sites.

An expression vector of the present invention can be transformed into any suitable host cell to form a recombinant cell. A suitable host cell includes any cell capable of expressing a nucleic acid molecule inserted into the expression vector. For example, a procaryotic expression vector can be transformed into a bacterial host cell. If the expression vector contains a T7 promoter then a source of T7 RNA polymerase must be provided to induce expression. Some host cells contain the T7 RNA polymerase gene in a repressed state. Expression of T7 RNA polymerase can be induced with a chemical signal such as IPTG or heat. Alternatively, a source of T7 RNA polymerase can be introduced at the appropriate time by infection with a phage containing a copy of T7 RNA polymerase. A wide range of hosts strains can be infected with a suitable phage. Some host strains have been engineered to contain inducible copies of T7 RNA polymerase gene. Such host strains include BL21(DE3) and derivatives thereof. A preferred host strain of the present invention is BL21(DE3)pLysS or BL21(DE3)pLysE, which are commercially available from Novagen and can be readily transformed with a DNA plasmid vector containing a MurG gene under the control of the T7 promoter. As already stated above, a preferred vector is a pET vector, preferably containing a restriction enzyme site permitting cloning of the gene as a fusion containing a C-terminal his tag.

In a preferred embodiment, one method to isolate MurG protein useful for producing MurG crystals includes recovery of MurG protein having a C-terminal LEHHHHHH (His tag) sequence purified as described in Ha et al. (1999, J. Amer. Chem. Soc. 121:8415-8426). One of skill in the art is able to modify this procedure in order to purify other proteins can be produced as C-terminal histadine (his) tags. The purification conditions for specific MurG proteins will vary depending upon the particular characteristics of the proteins such as their isoelectric point, molecular weight, etc. It is known that the isoelectric points of different MurG homologues vary a

bit, although they are generally relatively high. Also, some MurG homologues may be more hydrophobic than others, which will mean differences in amount of detergent necessary for purification. It is likely that all the MurG homologues can be purified over nickel affinity columns using the C-terminal his-tag as a handle. Those skilled in the art of protein purification will know how to modify purification parameters depending upon the protein characteristics, in order to purify the protein for crystallization.

STRUCTURE OF MurG PROTEIN

One embodiment of the present invention includes a model of a MurG protein, in which the model represents a three-dimensional structure of a MurG protein. Another embodiment of the present invention includes the three-dimensional structure of a MurG protein. A three-dimensional structure of a MurG protein encompassed by the present invention substantially conforms with the atomic coordinates represented in Table 1. According to the present invention, the use of the term "substantially conforms" refers to at least a portion of a three-dimensional structure of a MurG protein which is sufficiently spatially similar to at least a portion of a specified three-dimensional configuration of a particular set of atomic coordinates (e.g., those represented by Table 1) to allow the three-dimensional structure of another MurG protein to be modeled or calculated using the particular set of atomic coordinates defining the three-dimensional configuration of the MurG protein. For example, but not meant to be a limitation, homology modeling can be done using the linear sequence of a different MurG and *E. coli* coordinates; molecular replacement can allow the solution of a different MurG structure using the *E. coli* MurG coordinates and experimental data such as x-ray diffraction pattern from a different MurG crystal. According to the present invention, a three-dimensional structure of a given portion or chain of a first MurG protein can substantially conform to at least a portion of the atomic coordinates which represent a three-dimensional configuration of a second MurG.

More particularly, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of such structure has an average root-mean-square deviation (RMSD) of less than about 2.5 Å for the α-carbon or C-alpha backbone atoms in secondary structure elements in each domain, and more

preferably, less than about 2.0 Å for the C-alpha backbone atoms in secondary structure elements in each domain, and, in increasing preference, less than about 1.5 Å, less than about 1.0 Å, less than about 0.7 Å, and more preferably, less than about 0.5 Å for the C-alpha backbone atoms in secondary structure elements in each domain. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of such structure has the recited average root-mean-square deviation (RMSD) value, and more preferably, at least about 90% of such structure has the recited average RMSD value, and most preferably, about 100% of such structure has the recited average RMSD value.

In an even more preferred embodiment, the above definition of "substantially conforms" can be extended to include atoms of amino acid side chains. As used herein, the phrase "common amino acid side chains" refers to amino acid side chains that are common to both the structure which substantially conforms to a given set of atomic coordinates and the structure that is actually represented by such atomic coordinates. Preferably, a three-dimensional structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of the common amino acid side chains have an average RMSD value of less than about 1.5 Å, and more preferably, less than about 1.3 Å, and in increasing preference, less than about 1.0 Å, less than about 0.7 Å, and most preferably, less than about 0.3 Å.

In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of the common amino acid side chains have the recited average RMSD value, and more preferably, at least about 90% of the common amino acid side chains have the recited average RMSD value, and most preferably, about 100% of the common amino acid side chains have the recited average RMSD value.

In more preferred embodiments of the present invention, a large number of different "rotamers" or "rotational isomers" of the MurG protein are encompassed by three-dimensional structures of the invention in which the amino acid side chains are at a variety of positions in crystalline forms of the protein or for the protein in solution. Different rotamers refer to molecules of identical configuration may be distinguished as having different conformations after rotation about the various molecular bonds. Therefore, while the same or similar amino acids may be present, the exact location will

vary depending upon the freedom of rotation of the bonds due to hydrogen bonding, and other molecular forces.

STRUCTURE OF THE α-CARBON BACKBONE OF MurG AND THE α-CARBON BACKBONE AND CONSERVED AMINO ACID RESIDUES

The present invention includes the three-dimensional structure of the α-carbon or C-alpha backbone of a MurG protein, in particular the *E. coli* MurG protein. A three-dimensional structure of the C-alpha backbone of the MurG protein encompassed by the present invention substantially conforms with the atomic coordinates represented in Table 2.

More particularly, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of such structure has an average root-mean-square deviation (RMSD) of less than about 2.5 Å for the C-alpha backbone atoms in secondary structure elements in each domain, and more preferably, less than about 2.0 Å for the C-alpha backbone atoms in secondary structure elements in each domain, and, in increasing preference, less than about 1.5 Å, less than about 1.0 Å, less than about 0.7 Å, and more preferably, less than about 0.5 Å for the C-alpha backbone atoms in secondary structure elements in each domain. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of such structure has the recited average root-mean-square deviation (RMSD) value, and more preferably, at least about 90% of such structure has the recited average RMSD value, and most preferably, about 100% of such structure has the recited average RMSD value. The C-alpha backbone of MurG proteins is expected to be more conserved than the location of the particular amino acid residue side chains.

The present invention also includes the three-dimensional structure of the (α-carbon or C-alpha backbone and conserved or invariant amino acid residue side chains of a MurG protein, in particular the *E. coli* MurG protein. A three-dimensional structure of the C-alpha backbone and conserved amino acid residues of the MurG protein encompassed by the present invention substantially conforms with the atomic coordinates represented in Table 3. The conserved amino acids are highlighted in blue in Figure 3a and include G14, G15, G18, H19, G104, H124, E125, G190, G191, S192,

G194, A195, R261, G263, A264, E269, P281, Q289, N292 and A293 (as numbered in the *E. coli* MurG sequence set forth in Figure 3a).

More particularly, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of such structure has an average root-mean-square deviation (RMSD) of less than about 2.5 A, for the C-alpha backbone and conserved amino acid residue atoms in secondary structure elements in each domain, and more preferably, less than about 2.0 A for the backbone atoms in secondary structure elements in each domain, and, in increasing preference, less than about 1.5 A, less than about 1.0 A, less than about 0.7 A, and more preferably, less than about 0.5 A for the backbone atoms in secondary structure elements in each domain. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of such structure has the recited average rootmean-square deviation (RMSD) value, and more preferably, at least about 90% of such structure has the recited average RMSD value, and most preferably, about 100% of such structure has the recited average RMSD value.

STRUCTURE OF THE DONOR NUCLEOTIDE BINDING SITE OF MurG PROTEINS

An embodiment of the present invention includes the three-dimensional structure of a donor nucleotide binding site of a MurG protein, in particular an *E. coli* MurG protein. A more preferred embodiment of the present invention includes a three-dimensional structure of a donor nucleotide binding site of a MurG protein wherein the three-dimensional structure of the donor nucleotide binding site substantially conforms to the atomic coordinates in Table 4. In a preferred embodiment, the donor nucleotide binding site is a UDP-GlcNAc binding site of a MurG protein.

As described in Example 1, the donor nucleotide binding site is located in the C-terminal domain (see Fig. 4a). This binding site is based on the comparison of β-glucosyltransferase (BGT) and *E. coli* MurG and based on experiments done in our laboratory showing that the isolated C domain binds to a UDP-hexose column (See Example 1). The atomic coordinates of Table 4 set forth the donor nucleotide binding site three-dimensional structure without a donor nucleotide such as UDP-GlcNAc bound to the MurG protein.

According to the present invention, the use of the term "substantially conforms" refers to at least a portion of a three-dimensional structure of a donor nucleotide binding site of a MurG protein which is sufficiently spatially similar to at least a portion of a specified three-dimensional configuration of a particular set of atomic coordinates (e.g., those represented by Table 4) to allow the three-dimensional structure of the donor nucleotide binding domain to be modeled or calculated (i.e., by molecular replacement) using the particular set of atomic coordinates defining the three-dimensional configuration of the donor nucleotide binding site of a MurG protein. According to the present invention, a three-dimensional structure of a given donor nucleotide binding site of a first MurG protein can substantially conform to at least a portion of the atomic coordinates which represent a three-dimensional configuration of a second MurG. Since the atomic coordinates of Table 4 were obtained from the *E. coli* MurG crystal protein without a donor nucleotide bound, there will be some variation from the atomic coordinates of the donor nucleotide binding site when a nucleotide is bound vs. unbound. Therefore, a structure "substantially conforming" to that represented by the atomic coordinates in Table 4, will include a structure obtained from co-crytallization of the protein with a donor nucleotide.

More particularly, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of such structure has an average root-mean-square deviation (RMSD) of less than about 1.5 Å for the C-alpha backbone atoms in secondary structure elements in each domain, and more preferably, less than about 1.3 Å for the C-alpha backbone atoms in secondary structure elements in each domain, and, in increasing preference, less than about 1.0 Å, less than about 0.7 Å, and more preferably less than about 0.5 Å for the C-alpha backbone atoms in secondary structure elements in each domain. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of such structure has the recited average root-mean-square deviation (RMSD) value, and more preferably, at least about 90% of such structure has the recited average RMSD value.

In an even more preferred embodiment, the above definition of "substantially conforms" can be extended to include atoms of the conserved or invariant amino acid side chains located within the binding site. As used herein, the phrase "conserved

amino acid side chains" refers to amino acid side chains that are conserved between MurG proteins within the donor nucleotide binding site. The conserved amino acid residues of the donor nucleotide binding site have been identified as I125, R261, G263, A264, E269, P281, Q289, N292 and A293 (as numbered in the *E. coli* MurG sequence set forth in Figure 3a) and the G loop found between residues numbered 190-195 having residues G190, G191, S192, G194, and A195. Some or all of these conserved residues are necessary for binding the nucleotide donor.

Preferably, a three-dimensional structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of the conserved amino acid side chains have an average RMSD value of less than about 1.5 Å, and more preferably, less than about 1.3 Å, and in increasing preference, less than about 1.0 Å, less than about 0.7 Å, and most preferably, less than about 0.3 Å. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of the conserved amino acid side chains have the recited average RMSD value, and more preferably, at least about 90% of the conserved amino acid side chains have the recited average RMSD value, and most preferably, about 100% of the conserved amino acid side chains have the recited average RMSD value.

STRUCTURE OF THE ACCEPTOR BINDING SITE OF MurG PROTEIN

An embodiment of the present invention includes the three-dimensional structure of an acceptor binding site of a MurG protein. A three-dimensional structure of a acceptor binding site of a MurG protein encompassed by the present invention substantially conforms with the atomic coordinates represented in Table 5. A more preferred embodiment of the present invention includes a three-dimensional structure of an acceptor binding site of a MurG protein wherein the three dimensional structure of the acceptor binding site substantially conforms to the atomic coordinates Table 5.

According to the present invention, the use of the term "acceptors" refers to Lipid I and analogues thereof. For the purposes of obtaining co-crystals containing acceptor analogues bound to the acceptor binding site better, the analogues need not be functional acceptors in a MurG assay. In particular embodiments of the present invention, the acceptor is selected from the group consisting of, but not limited to

Lipid I, and analogs of Lipid I (see compounds described in Ha et al., J. Amer. Chem. Soc. 1999, vol. 121:8415-26, incorporated by herein by reference in its entirety).

As described in Example 1, the acceptor binding site is located in the N-terminal domain of a MurG protein (see Fig. 3a and 4c). The acceptor binding site or domain is characterized by three highly conserved regions, twp of which are glycine-rich loops (also referred to as "G loops") that face the cleft between the C-terminal and N-terminal domains. The conserved residues of the acceptor binding site comprise G14, G15, G18, H19, G104, H124, and E125 (as numbered in the *E. coli* MurG sequence set forth in Figure 3a) and two conserved G loop structures.

According to the present invention, the use of the term "substantially conforms" refers to at least a portion of a three-dimensional structure of an acceptor binding site of a MurG protein which is sufficiently spatially similar to at least a portion of a specified three-dimensional configuration of a particular set of atomic coordinates (e.g., those represented by Table 5) to allow the three-dimensional structure of the acceptor binding site to be modeled or calculated (i.e., by homology modeling) using the particular set of atomic coordinates defining the three-dimensional configuration of the acceptor binding site of a MurG protein. According to the present invention, a three-dimensional structure of a given acceptor binding site of a first MurG protein can substantially conform to at least a portion of the atomic coordinates which represent a three-dimensional configuration of a second MurG.

In an even more preferred embodiment, the above definition of "substantially conforms" can be extended to include atoms of the conserved amino acid side chains. As used herein, the phrase "conserved amino acid side chains" refers to the conserved or invariant amino acid side chains that are common to MurG proteins. Preferably, a three-dimensional structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of the conserved amino acid side chains have an average RMSD value of less than about 1.5 Å, and more preferably, less than about 1.3 Å, and in increasing preference, less than about 1.0 Å, less than about 0.7 Å, and most preferably, less than about 0.3 Å. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of the conserved amino acid side chains have the recited average RMSD value, and more preferably, at least about 90% of the conserved amino

acid side chains have the recited average RMSD value, and most preferably, about 100% of the conserved amino acid side chains have the recited average RMSD value.

STRUCTURE OF A MEMBRANE ASSOCIATION SITE OF MurG PROTEIN

An embodiment of the present invention includes the three-dimensional structure of a membrane association site of a MurG protein. A three-dimensional structure of a membrane association site of a MurG protein encompassed by the present invention substantially conforms with the atomic coordinates represented in Table 6. A more preferred embodiment of the present invention includes a three-dimensional structure of an acceptor binding site of a MurG protein wherein the three-dimensional structure of the acceptor binding site substantially conforms to the atomic coordinates in Table 6.

According to the present invention, the use of the term "membrane association site" refers to the region of a MurG protein that associates with cytoplasmic surface of bacterial membranes where it performs the reaction of coupling a soluble donor sugar to the membrane anchored acceptor sugar, Lipid I. Analysis of the *E. coli* MurG protein structure shows a hydrophobic patch consisting of residues 175, L79, F82, W85, and W116 in the N-domain. The membrane association site is where the MurG protein associates with the bacterial membranes, and that it is target for inhibitors if we find that a) we can bind to it with another molecule; b) we can disrupt membrane association by binding to it; or c) disrupting membrane association inhibits activity.

As described in Example 1, the membrane association site is located in the N-terminal domain of a MurG protein (see Fig. 4c). The location of the membrane association site is in close proximity to the acceptor binding site and membrane association in this patch would bring the two M-terminal G-loops close to the membrane surface where the diphosphate portion of the acceptor is located.

According to the present invention, the use of the term "substantially conforms" refers to at least a portion of a three-dimensional structure of a membrane association site of a MurG protein which is sufficiently spatially similar to at least a portion of a specified three-dimensional configuration of a particular set of atomic coordinates (e.g., those represented by Table 6) to allow the three-dimensional structure of the membrane association site to be modeled or calculated (i.e., by molecular replacement) using the particular set of atomic coordinates defining the three-dimensional configuration of the

membrane association site of a MurG protein. According to the present invention, a three-dimensional structure of a given membrane association site of a first MurG protein can substantially conform to at least a portion of the atomic coordinates which represent a three-dimensional configuration of a second MurG.

More particularly, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of such structure has an average root-mean-square deviation (RMSD) of less than about 1.5 Å for the structural elements in the site, and more preferably, less than about 1.3 Å for the structure elements in each site, and, in increasing preference, less than about 1.0 Å, less than about 0.7 Å, less than about 0.5 Å, and more preferably, less than about 0.3 Å for the structural elements in each site. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of such structure has the recited average root-mean-square deviation (RMSD) value, and more preferably, at least about 90% of such structure has the recited average RMSD value, and most preferably, about 100% of such structure has the recited average RMSD value.

In an even more preferred embodiment, the above definition of "substantially conforms" can be extended to include atoms of α-carbon backbone and conserved amino acid side chains. As used herein, the phrase "conserved amino acid side chains" refers to amino acid side chains that are conserved between MurG proteins. Preferably, a three-dimensional structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of the conserved α-carbon backbone and conserved amino acid side chains have an average RMSD value of less than about 1.5 Å, and more preferably, less than about 1.3 Å, and in increasing preference, less than about 1.0 Å, less than about 0.7 Å, and most preferably, less than about. 0.3 Å. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of the α-carbon backbone and conserved amino acid side chains have the recited average RMSD value, and more preferably, at least about 90% of the α-carbon backbone and conserved acid side chains have the recited average RMSD value, and most preferably, about 100% of the α-carbon and conserved amino acid side chains have the recited average RMSD value.

COMPUTER READABLE MEDIUM

Another embodiment of the present invention relates to a computer-readable medium encoded with a set three-dimensional coordinates seleceted from the group consisting of the three-dimensional coordinates represented in Table 1, the three-dimensional coordinates represented in Table 2, the three-dimensional coordinates represented in Table 3, the three-dimensional coordinates represented in Table 4, the three-dimensional coordinates represented in Table 5, or the three-dimensional coordinates represented in Table 6, wherein using a graphical display software program, the three-dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three-dimensional image. Preferably, the three-dimensional image is of a MurG protein, the α-carbon backbone of MurG, the α-carbon backbone and conserved amino acid residue sidechains of MurG, the donor nucleotide binding site of MurG, the acceptor binding site of MurG, or the membrane association site of MurG.

Yet another embodiment of the present invention relates to a computer-readable medium encoded with a set of three-dimensional coordinates of a three-dimensional structure which substantially conforms to the three-dimensional coordinates represented in Table 1, wherein using a graphical display software program, the three-dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three-dimensional image. In other embodiments, the present invention relates to a computer-readable medium encoded with a set of three-dimensional coordinates of a three-dimensional structure which substantially conforms to the three-dimensional coordinates represented in Table 2, Table 3, Table 4, Table 5 or Table 6, wherein using a graphical display software program, the three-dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three-dimensional image. Preferably, the three-dimensional image is of a MurG protein, the α-carbon backbone of MurG, the α-carbon backbone and conserved amino acid residue sidechains of MurG, the donor nucleotide binding site of MurG, the acceptor binding site of MurG, or the membrane association site of MurG.

IMAGES

One embodiment of the present invention relates to a two dimensional image of an *E. coli* MurG protein including those illustrated in Figures 3-4. Most of these figures were drawn with the MOLSCRIPT program. Preferably, the two dimensional image is of a MurG protein, the α-carbon backbone of MurG, the α-carbon backbone and conserved amino acid residue sidechains of MurG, the donor nucleotide binding site of MurG, the acceptor binding site of MurG, or the membrane association site of MurG.

Another embodiment of the present invention includes a three-dimensional computer image of the three-dimensional structure of a MurG protein, preferably the *E. coli* MurG protein. Suitable structures of which to produce three-dimensional computer images are disclosed herein. Preferably, a computer image is created to a structure substantially conforming with the three-dimensional coordinates represented in Table 1.

Another embodiment of the present invention includes an image of an MurG protein that is generated when a set of three-dimensional coordinates comprising the three-dimensional coordinates represented in Table 1 are analyzed on a computer using a graphical display software program to create an electronic file of the image and visualizing the electronic file as a three-dimensional image. Suitable structures to image are disclosed herein. Preferably, the three-dimensional structures are of a MurG protein, the α-carbon backbone of MurG, the α-carbon backbone and conserved amino acid residue sidechains of MurG, the donor nucleotide binding site of MurG, the acceptor binding site of MurG, or the membrane association site of MurG. Most preferably, the MurG protein is the *E. coli* MurG protein described herein. A computer image of the present invention can. be produced using any suitable software program, including, but not limited to, MOLSCRIPT 2.0 (Avatar Software AB, Helenebrgsgatan 21 C, SE-11713, Stockholm, Sweden), the graphical display program O (Jones et al., Acta Crystallography, vol. A47, p. 110, 1991), or the graphical display program GRASP. Suitable computer hardware useful for producing an image of the present invention are known to those of skill in the art. Preferred computer hardware includes a Silicon Graphics Workstation.

MODELS OF MurG PROTEINS AND BINDING SITES

According to the present invention, a three-dimensional structure of the *E. coli* MurG protein and its binding sites of the present invention can be used to derive a model of the three-dimensional structure of another MurG protein and its binding sites (i.e., a structure to be modeled). As used herein, a "structure" of a protein refers to the components and the manner of arrangement of the components to constitute a protein or binding site. Also, as used herein, the term "model" refers to a representation of a tangible medium of the three-dimensional structure of a protein, polypeptide or peptide, or binding site of a protein. For example, a model can be a representation of the three-dimensional structure in a electronic file, on a computer screen, on a piece of paper (i.e., on a two dimensional medium), and/or as a ball-and-stick figure. Physical three-dimensional models are tangible and include, but are not limited to, stick models and space-filling models. The phrase "imaging the model on a computer screen" refers to the ability to express (or represent) and manipulate the model on a computer screen using appropriate computer hardware and software technology known to those skilled in the art. Such technology is available from a variety of sources including, for example, Evans and Sutherland, Salt Lake City, Utah, and Biosym Technologies, San Diego, CA. The phrase "providing a picture of the model" refers to the ability to generate a "hard copy" of the model. Computer screen images and pictures of the model can be visualized in a number of formats including space-filling representations, α-carbon traces, ribbon diagrams and electron density maps.

Suitable target MurG proteins and their associated binding sites to model using a method of the present invention include any MurG protein and binding sites that are at least in part structurally related to the *E. coli* MurG protein or its binding sites. A preferred target MurG structure that is at least in part structurally related includes a target MurG structure having an amino acid sequence that is at least about 25%, preferably at least about 30%, more preferably at least about 36%, more preferably at least about 40%, even more preferably at least about 50%, more preferably at least about 60%, more preferably at least about 70%, more preferably at least about 80%, and more preferably at least about 90% identical to an amino acid sequence of the *E. coli* MurG protein, across the full-length of the target MurG structure sequence when using, for example, a sequence alignment program such as DNAsis™ program (available from

Hitachi Software, San Bruno, CA) or the MacVector™ program (available from the Eastman Kodak Company, New Haven, CT) or the GCγ ™ program (available from the "GCγ ", University of Wisconsin, Madison, WI), such alignment being performed for example, using the standard default values accompanying such alignment programs.

Preferred MurG proteins and their binding sites are set forth in the amino acid sequences of MurG proteins as deposited in the NCBI database and are identified with Accession Nos. CAB51993, A71316, E70579, C71699, F70195, A43727, JC1275, BVECMG, CEECAM, 083535, Q9ZK59, CAB85280, AAF39020, BAA18775, AAD26629, CAB73295, P37585, Q9ZHA9, Q9ZHDC0, Q9ZBA5, Q9X4H4, Q9WY74, P74657, O06224, Q9Z702, O84766, O69552, O67238, O51708, O25770, O07670, O07109, P45065, CAB66324, AAC68356, AAF06830, P18579, P17443, P17952, P16457, P07862, AAE23178, AAD53936, CAA18668, CAA38869, CAA38868, CAA38867, CAA38866, AAD08196, BAA01453, BAA01455, BAA01454, AAD19042, CAA45558, CAA74235, AAD10537, AAD06652, AAC95450, CAA14869, AAC73201, AAC65509, AAC67113, AAC45636, CABO8640, AAC22793, AAC07193, BAA24357, CAB13395, BAA01355, AAB35538, 1904153C, 1808265B, 1808265A, CAA36866, CAA36869, CAA36868, CAA36867, CAA36776, and AAA99436. The amino acid sequences are publicly available.

A variety of MurG proteins from numerous organisms can be used to prepare models of MurG proteins and binding sites, including but not limited to, microorganisms such as bacteria, higher-order bacteria, thermal stable bacteria, spirochetes, small pathogenic organisms, fungi, protozoa, cyanobacteria, and trypanosomes. More particularly, bacteria such as but not limited to, *Escherichia coli, Bacillus subtilis, Aquefex aeolicus, Borrelia burgdorferi, Chlamydia pneumoniae, Chlamydia trachomatis, Enterococcus faecais, Enterococcus hirae, Haemophilus influenzae, Helicobacter pyloir J99 , Helicobacter pylori, Mycobacterium tuberculosis, Porphyromonas gingivalis, Rickettsia prowazekii, Streptomyces coelicolor, Streptomyces collinus, Streptococcus pneumoniae, Synechocystis* sp. (strain PCC6803), *Thermotoga maritime,* and *Treponema pallidum*. It is noted that nucleotide and amino acid sequences for many of the above identified organisms are known and publicly available.

Preferred target MurG proteins and binding site structures to model also include, but are not limited to, derivatives of MurG proteins, such as a MurG protein having one or more amino acid residues substituted, deleted or added (referred to herein as MurG mutants), or proteins encoded by natural variants of a nucleic acid molecule encoding a MurG.

In another embodiment of the invention, the process of building a homology model for a protein is divided into the following steps:

(1) Determine which proteins are related to the model protein;

(2) Determine structurally conserved regions (SCRs);

(3) Align the amino acid sequence of the unknown protein with those of the reference protein(s) within the SCRs;

(4) Assign coordinates in the conserved regions;

(5) Predict conformations for the rest of the peptide chain, including loops between the SCRs and possibly the N- and C-termini;

(6) Search for the optimum side chain conformations for residues that differ from those in the reference proteins; and

(7) Use energy minimization and molecular dynamics to refine the molecular structure so that steric strain introduced during the model-building process can be relieved.

Published sequences are readily available through on-line databases on the Internet, such as SwissProt (http://www.expasy.ch/sprot/sprot-top.html). MurG specific and related sequences are obtained for use for building homology models by text-based or sequence similarity searching. SCRs for MurG is the entire protein, considering the *E. coli* MurG crystal structure is the only similar sequence with structural data. Alignment of the sequences using an appropriate alignment program and algorithm, such as Clustal W, allows appropriate assignment of the *E. coli* protein coordinates to a MurG sequence of unknown structure. The Modeler program performs the conformational predictions for the peptide chain and side chains. Dynamics and minimization using an appropriate program and algorithm, such as Discover.

Modeler Description:

Modeler is an automated homology-modeling scheme designed to find the most probable three-dimensional structure of a protein, given its amino acid sequence and its

alignment with related structures. It derives 3D protein models without the time consuming separate stages of core region identification and loop region building or searching that is inherent to manual homology modeling schemes. The related or reference protein structures are used to derive spatial restraints expressed as probability density functions (PDFs) for each of the restrained features of the model. As an example, the main chain conformation of a given residue in the model will be described by restraints that depend upon the residue type, the main chain conformation of equivalent residues in the reference proteins and the local sequence similarity. The probability distribution functions that are used in restraining the model structure are derived from correlations between structural features in a database of families of homologous proteins aligned on the basis of their 3D structure. These functions are used to restrain C-C distances, main chain N--O distances, main chain and side chain dihedral angles, etc. The individual restraints are assembled into a single molecular probability density function (MPDF). The three-dimensional protein model is then obtained by an optimization of this MPDF. The optimization procedure itself consists of a variable target function method (Braun and Go, 1985) with conjugate gradient minimization scheme followed by an optional restrained simulated annealing molecular dynamics scheme.

While several reference structures are used in the traditional homology model building process, only one set of coordinates can be used in any one peptide segment. Modeler is able to simultaneously incorporate structural data from one or more reference proteins. Structural features in the reference proteins are used to derive spatial restraints which in turn are used to generate model protein structures using conjugate gradient and simulated annealing optimization procedures.

Clustal W description:

Clustal W aligns multiple sequences using a progressive pairwise alignment algorithm. It first generates all possible pairwise alignments for a list of sequences and then builds the guide tree based on their pairwise sequence identity, aligning the sequences following the order of the guide tree.

Several unique features in Clustal W improve the sensitivity of the alignment of divergent protein sequences (Thompson et al, 1994a).

(1) Individual weights are assigned to each sequence in a partial alignment in order to downweight near-duplicate sequences and upweight the most divergent ones.

(2) Amino acid substitution matrices are varied at different alignment stages according to the divergence of the sequences to be aligned.

(3) Residue-specific gap penalties and locally reduced gap penalties in hydrophilic regions encourage new gaps in potential loop regions rather than regular secondary structure.

(4) Positions in early alignments, where gaps have been opened, receive locally reduced gap penalties to encourage the opening of new gaps at these positions.

Discover Description:

The Discover program performs energy minimization, template forcing, torsion forcing, and dynamic trajectories and calculates properties such as interaction energies, derivatives, mean square displacements, and vibrational frequencies. It provides tools for performing simulations under various conditions including constant temperature, constant pressure, constant stress, periodic boundaries, and fixed and restrained atoms.

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STRUCTURE BASED DRUG DESIGN

The present invention relates to the use of the crystal structure of the *E. coli* MurG protein represented by the atomic coordinates in Table 1 to make models of MurG proteins and binding sites thereof. The present invention also relates to the use of the crystal structure, α-carbon backbone, α-carbon backbone plus conserved amino acid residue side chains or binding sites of the *E. coli* MurG protein to construct models of these structures in other MurG proteins.

For the first time, the present invention permits the use of molecular design techniques to design, select and synthesize chemical entities and compounds, including inhibitory compounds, capable of binding to the active site or accessory binding site of MurG, in whole or in part.

On approach enabled by this invention, is to use the structure coordinates of MurG to design compounds that bind to the enzyme and alter the physical properties of the compounds in different ways, e.g., solubility. For example, this invention enables the design of compounds that act as inhibitors of the MurG enzyme by binding to, all or a portion of, the active site of MurG.

A second design approach is to probe a MurG crystal with molecules composed of a variety of different chemical entities to determine optimal sites for interaction between candidate MurG inhibitors and the enzyme. For example, high resolution X-ray diffraction data collected from crystals saturated with solvent allows the determination of where each type of solvent molecule sticks. Small molecules that bind

tightly to those sites can then be designed and synthesized and tested for their MurG inhibitor activity. Travis, J., Science, 262, p. 1374 (1993).

This invention also enables the development of compounds that can isomerize to short-lived reaction intermediates in the chemical reaction of a substrate or other compound that binds to MurG, with MurG. Thus, the time-dependent analysis of structural changes in MurG during its interaction with other molecules is enabled. The reaction intermediates of MurG can also be deduced from the reaction product in co-complex with MurG. Such information is useful to design improved analogues of known MurG inhibitors or to design novel classes of inhibitors based on the reaction intermediates of the MurG enzyme and MurG-inhibitor co-complex. This provides a novel route for designing MurG inhibitors with both high specificity and stability.

Another approach made possible and enabled by this invention, is to screen computationally small molecule data bases for chemical entities or compounds that can bind in whole, or in part, to the MurG enzyme. In this screening, the quality of fit of such entities or compounds to the binding site may be judged either by shape complementarity or by estimated interaction energy. Meng, E. C. et al., J. Coma. Chem., 13, pp.505-524 (1992).

Because MurG may crystallize in more than one crystal form, the structure coordinates of MurG, or portions thereof, as provided by this invention are particularly useful to solve the structure of those other crystal forms of MurG. They may also be used to solve the structure of MurG mutants, MurG co-complexes, or of the crystalline form of any other protein with significant amino acid sequence homology to any functional domain of MurG.

One method that may be employed for this purpose is molecular replacement. In this method, the unknown crystal structure, whether it is another crystal form of MurG a MurG mutant, or a MurG co-complex, or the crystal of some other protein with significant amino acid sequence homology to any functional domain of MurG, may be determined using the MurG structure coordinates of this invention as provided in Tables 1-6. This method will provide an accurate structural form for the unknown crystal more quickly and efficiently than attempting to determine such information ab initio.

In addition, in accordance with this invention, MurG mutants may be crystallized in co-complex with known MurG inhibitors. The crystal structures of a series of such complexes may then be solved by molecular replacement and compared with that of wild-type MurG. Potential sites for modification within the various binding sites of the enzyme may thus be identified. This information/provides an additional tool for determining the most efficient binding interactions, for example, increased hydrophobic interactions, between MurG and a chemical entity or compound.

All of the complexes referred to above may be studied using well-known X-ray diffraction techniques and may be refined versus 2-3 .ANG. resolution X-ray date to an R value of about 0.20 or less using computer software, such as X-PLOR (Yale University, .COPYRGT.1992, distributed by Molecular Simulations, Inc.). See, e.g., Blundel & Johnson, supra; Methods in Enzvmoloav, vol. 114 & 115, H. W. Wyckoff et al., eds., Academic Press (1985). This information may thus be used to design, synthezie and optimize novel classes of MurG inhibitors.

The structure coordinates of MurG mutants provided in this invention also facilitate the identification of related proteins or enzymes analogous to MurG in function, structure or both, thereby further leading to novel therapeutic modes for treating or preventing UDP-glycosyltransferase mediated diseases.

The design of compounds that bind to or inhibit MurG according to this invention generally involves consideration of two factors. First, the compound must be capable of physically and structurally associating with MurG. Non-covalent molecular interactions important in the association of MurG with its substrate include hydrogen bonding, van der Waals and hydrophobic interactions.

Second, the compound must be able to assume a conformation that allows it to associate with MurG. Although certain portions of the compound will not directly participate in this association with MurG, those portions may still influence the overall conformation of the molecule. This, in turn, may have a significant impact on potency. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical entity or compound in relation to all or a portion of the binding site, e.g., active site or accessory binding site of MurG, or the spacing between functional groups of a compound comprising several chemical entities that directly interact with MurG.

The potential inhibitory or binding effect of a chemical compound on MurG may be analyzed prior to its actual synthesis and testing by the use of computer modelling techniques. If the theoretical structure of the given compound suggests insufficient interaction and association between it and MurG, synthesis and testing of the compound is obviated. However, if computer modelling indicates a strong interaction, the molecule may then be synthesized and tested for its ability to bind to MurG and inhibit using the assay of Walker et al. patents (cited supra). In this manner, synthesis of inoperative compounds may be avoided.

An inhibitory or other binding compound of MurG may be computationally evaluated and designed by means of a series of steps in which chemical entities or fragments are screened and selected for their ability to associate with the individual binding pockets or other areas of MurG.

One skilled in the art may use one of several methods to screen chemical entities or fragments for their ability to associate with MurG and more particularly with the individual binding pockets of the MurG donor nucleotide binding site, acceptor binding site or membrane association site. This process may begin by visual inspection of, for example, the binding sites on the computer screen based on the MurG coordinates in Tables 1-6. Selected fragments or chemical entities may then be positioned in a variety of orientations, or docked, within an individual binding pocket of MurG as defined supra. Docking may be accomplished using software such as Quanta and Sybyl, followed by energy minimization and molecular dynamics with standard molecular mechanics forcefields, such as CHARMM and AMBER.

Specialized computer programs may also assist in the process of selecting fragments or chemical entities, including but not limited to:

1. GRID (Goodford, P. J., "A Computational Procedure for Determining Energetically Favorable Binding Sites on Biologically Important Macromolecules" J. Med. Chem., 28, pp.849-857 (1985)). GRID is available &orn Oxford University, Oxford, UK.

2. MCSS (Miranker, A. and M. Karplus, "Functionality Maps of Binding Sites: A Multiple Copy Simultaneous Search Method." Proteins: Structure, Function and Genetics, 11, pp.29-34 (1991)). MCSS is available from Molecular Simulations, Burlington, Mass.

3. AUTODOCK (Goodsell, D. S. and A. J. Olsen, "Automated Docking of Substrates to Proteins by Simulated Annealing" Proteins: Structure. Function, and Genetics, 8, pp.195-202 (1990)) (AUTODOCK is available from Scripps Research Institute, La Jolla, Calif.).

4. DOCK (Kuntz, I. D. et al., "A Geometric Approach to Macromolecule-Ligand Interactions" J. Mol. Biol., 161, pp.269-288 (1982)). DOCK is available from University of California, San Francisco, Calif.

Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound or inhibitor. Assembly may be proceeded by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of MurG. This would be followed by manual model building using software such as Quanta or Sybyl.

Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include, but are not limited to:

1. CAVEAT (Bartlett, P. A. et al, "CAVEAT: A Program to Facilitate the Structure-Derived Design of Biologically Active Molecules". In Molecular Recognition in Chemical and Biological Problems", Special Pub., Royal Chem. Soc., 78, pp.182-196 (1989)). CAVEAT is available from the University of California, Berkeley, Calif.

2. 3D Database systems such as MACCS-3D (MDL Information Systems, San Leandro, Calif). This area is reviewed in Martin, Y. C., "3D Database Searching in Drug Design", J. Med. Chem., 35, pp.2145-2154 (1992)).

3. HOOK (available from Molecular Simulations, Burlington, Mass.).

Instead of proceeding to build a MurG inhibitor in a step-wise fashion one fragment or chemical entity at a time as described above, inhibitory or other MurG binding compounds may be designed as a whole or "de novo" using either an empty active site or optionally including some portion(s) of a known inhibitor(s). These methods include, but are not limited to:

1. LUDI (Bohm, H.-J., "The Computer Program LUDI: A New Method for the De Novo Design of Enzyme Inhibitors", J. ComR. Aid. Molec. Design, 6, pp.61-78 (1992)). LUDI is available from Biosym Technologies, San Diego, Calif.

2. LEGEND (Nishibata, Y. and A. Itai, Tetrahedron, 47, p. 8985 (1991)). LEGEND is available from Molecular Simulations, Burlington, Mass.

3. LeapFrog (available from Tripos Associates, St. Louis, Mo.).

Other molecular modeling techniques may also be employed in accordance with this invention. See, e.g., Cohen, N. C. et al., "Molecular Modeling Software and Methods for Medicinal Chemistry", J. Med. Chem., 33, pp.883-894 (1990). See also, Navia, M. A. and M. A. Murcko, "The Use of Structural Information in Drug Design", Current Opinions in Structural Biology, 2, pp. 202-210 (1992).

Once a compound has been designed or selected by the above methods, the efficiency with which that compound may bind to MurG may be tested and optimized by computational evaluation. For example, a compound that has been designed or selected to function as a MurG-inhibitor must also preferably traverse a volume not overlapping that occupied by the active site when it is bound to the native substrate. An effective MurG inhibitor must preferably demonstrate a relatively small difference in energy between its bound and free states (i.e., a small deformation energy of binding). Thus, the most efficient MurG inhibitors should preferably be designed with a deformation energy of binding of not greater than about 10 kcal/mole, preferably, not greater than 7 kcal/mole. MurG inhibitors may interact with the enzyme in more than one conformation that is similar in overall binding energy. In those cases, the deformation energy of binding is taken to be the difference between the energy of the free compound and the average energy of the conformations observed when the inhibitor binds to the enzyme.

A compound designed or selected as binding to MurG may be further computationally optimized so that in its bound state it would preferably lack repulsive electrostatic interaction with the target enzyme. Such non-complementary (e.g., electrostatic) interactions include repulsive charge-charge, dipole-dipole and charge-dipole interactions. Specifically, the sum of all electrostatic interactions between the inhibitor and the enzyme when the inhibitor is bound to MurG, preferably make a neutral or favorable contribution to the enthalpy of binding.

Specific computer software is available in the art to evaluate compound deformation energy and electrostatic interaction. Examples of programs designed for such uses include, but are not limited to: Gaussian 92, revision C [M. J. Frisch,

Gaussian, Inc., Pittsburgh, Pa. COPYRIGHT. 1992]; AMBER, version 4.0 [P. A. Kollman, University of California at San Francisco, COPYRIGHT. 1994]; QUANTA/CHARMM [Molecular Simulations, Inc., Burlington, Mass. COPYRIGHT. 1994]; and Insight II/Discover (Biosysm Technologies Inc., San Diego, Calif COPYRIGHT. 1994). These programs may be implemented, for instance, using a Silicon Graphics workstation, IRIS Octane or IBM RISC/6000 workstation. Other hardware systems and software packages will be known to those skilled in the art.

Once a MurG-binding compound has been optimally selected or designed, as described above, substitutions may then be made in some of its atoms or side groups in order to improve or modify its binding properties. Generally, initial substitutions are conservative, i.e., the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group. It should, of course, be understood that components known in the art to alter conformation should be avoided. Such substituted chemical compounds may then be analyzed for efficiency of fit to MurG by the same computer methods described in detail, above.

COMPOUNDS AND COMPOSITIONS COMPRISING COMPOUNDS DERIVED FROM STRUCTURE BASED DRUG DESIGN

One embodiment of the present invention is a compound that is capable of binding to a MurG protein, inhibiting the activity of a MurG protein, or stimulating the activity of a MurG protein. Suitable inhibitory compounds of the present invention can: (1) inhibit (i.e., prevent or block) the activity of MurG enzyme by binding to a MurG donor nucleotide binding site and interfering with the binding of the donor nucleotide molecule; (2) inhibit the activity of MurG enzyme by binding to the MurG acceptor binding site and interfering with the binding of the acceptor molecule; (3) inhibit the activity of a MurG enzyme by binding to the membrane association site and interfering with the association of the protein with the bacterial membrane and/or acceptor molecule.

Another embodiment of the present invention is a compound that is capable of stimulating MurG activity. Suitable stimulatory compounds of the present invention can stimulate the activity of a MurG enzyme by binding to the protein at a binding site and causing an increase in enzymatic activity, for example, by increasing the enzymes

affinity to bind a donor nucleotide, an acceptor molecule or improve the enzymes stability or increasing the binding affinity of a molecule to MurG.

Such compounds that bind to, inhibit or stimulate activity of a MurG protein include, for example, compounds that mimic donor nucleotide molecules. In preferred embodiments, the compound includes, for example, pyrimidine nucleoside analogues. In yet another preferred embodiment, the compounds include compounds comprising a pyrimidine nucleoside with a substituent containing at least one heteroatom attached to the C5 hydroxyl. In more particular embodiments, pyrimidine derivatives make complementary hydrogen bonding contacts to the amide backbone segment containing Ile 245 and also contact glutamate 269.

Another embodiment of the present invention is a compound that binds to the acceptor binding site of the MurG protein, hereinafter referred to a acceptor analogs. An acceptor analog refers to a compound that interacts with (e.g., binds to, associates with, modifies) the acceptor binding site of a MurG protein. An acceptor analog, for example, is a compound that mimics the natural acceptor molecule, Lipid I. Examples of such acceptor analogs are set forth in Ha et al., J. Amer. Chem. Soc. 1999, and PCT/US99/02187, U.S. Provisional Application No. 60/073,376 filed February 2, 1998, incorporated herein by reference.

Another embodiment of the present invention is a compound that binds to the MurG protein, that are enzyme product analogs, hereinafter referred to as Lipid II analogs. A Lipid II analog refers to a compound that interacts with (i.e., binds to, associates with, modifies) the acceptor binding site of a Mur G protein which mimics the product of the transglycosylase reaction.

Inhibitory and stimulatory compounds of the present invention can be identified by various means known to those of skill in the art. For example, binding of an inhibitory compound to, or otherwise interaction with, a MurG protein, can be determined with MurG in solution, for example, using assays described in PCT/US99/02187, U.S. Provisional Application No. 60/073,376 filed February 2, 1998, and PCT/US00/05554 , U.S. Provisional Application Nos. 60/122,966 and 60/137,696, incorporated herein by reference.

According to the present invention, suitable compounds of the present invention include peptides or other organic molecules, and inorganic molecules. Suitable organic

molecules include small organic molecules. Preferably, a compound of the present invention is not harmful (i.e., toxic) to an animal when administered to an animal.

Compounds of the present invention also can be identified using structure based drug design techniques known to those skilled in the art and described herein above.

Also according to the present invention, compounds are suitable for use in the inhibition of bacterial or microbial growth in an animal, and for example, function as an antibiotic for treatment of bacterial infections in animals.

The present invention also includes compositions comprising compounds of the present invention that inhibit or stimulate MurG activity which function as antibiotics or antimicrobial agents in animals. Compositions of the present invention can be used therapeutically or diagnostically in an animal. Compositions of the present invention comprises at least one compound of the present invention. In a preferred embodiment, compositions of the present invention further comprise a carrier. More particularly, a suitable carrier is a pharmaceutically acceptable carrier known to those skilled in the art.

TABLE 1- ATOMIC COORDINATES OF E. COLI MURG PROTEIN

REMARK coordinates from minimization refinementREMARK refinement resolution: 40.0 - 1.9 AREMARK starting r= 0.2200 free_r= 0.2466REMARK final r= 0.2200 free_r= 0.2466REMARK rmsd bonds= 0.005558 rmsd angles= 1.29505REMARK wa= 1.08391REMARK target= mlf cycles= 1 steps= 30REMARK sg= P1 a= 60.613 b= 66.356 c= 67.902 alpha= 64.294 beta= 83.520 gamma= 65.448REMARK parameter file 1 :
CNS_TOPPAR:protein_rep.paramREMARK parameter file 2 :
CNS_TOPPAR:water_rep.paramREMARK parameter file 3 :
CNS_TOPPAR:ion.paramREMARK molecular structure file: gen.mtfREMARK input coordinates: gen.pdbREMARK reflection file= native.cvREMARK ncs= noneREMARK B-correction resolution: 6.0 - 1.9REMARK initial B-factor correction applied to fobs :REMARK B11= 0.747 B22= 2.098 B33= -2.845REMARK B12= -1.847 B13= -3.752 B23= 6.401REMARK B-factor correction applied to coordinate array B: 0.038REMARK bulk solvent: density level= 0.351665 e/A^3, B-factor= 43.8282 A^2REMARK reflections with |Fobs|/sigma_F < 2.0 rejectedREMARK reflections with |Fobs| > 10000 * rms(Fobs) rejectedREMARK theoretical total number of refl. in resol. range:68102 (100.0%)REMARK number of unobserved reflections (no entry or |F|=0):2825(4.1%) REMARK number of reflections rejected: 3288 (4.8 %)REMARK total number of reflections used: 61989 91.0%)REMARK number of reflections in working set: 55765 (81.9%)REMARK number of reflections in test set: 6224 (9.1%)CRYST1 60.613 66.356 67.902 64.29 83.52 65.45 P 1
REMARK FILENAME="minimize5.pdb"REMARK DATE:14-Jan-00 15:25:36 created by user: shaREMARK VERSION: 0.5

ATOM	1	CB	LYS	A	7	0.142	3.434	35.023	1.00	43.02	AAAA
ATOM	2	CG	LYS	A	7	1.076	4.457	35.641	1.00	46.34	AAAA
ATOM	3	CD	LYS	A	7	0.452	5.841	35.634	1.00	47.39	AAAA
ATOM	4	CE	LYS	A	7	1.345	6.846	36.332	1.00	48.65	AAAA
ATOM	5	NZ	LYS	A	7	0.780	8.221	36.276	1.00	51.04	AAAA
ATOM	6	C	LYS	A	7	-2.239	2.733	34.833	1.00	39.64	AAAA
ATOM	7	O	LYS	A	7	-2.050	1.717	34.160	1.00	39.64	AAAA
ATOM	8	N	LYS	A	7	-0.974	2.320	36.947	1.00	42.05	AAAA
ATOM	9	CA	LYS	A	7	-1.170	3.245	35.788	1.00	41.31	AAAA
ATOM	10	N	ARG	A	8	-3.357	3.451	34.773	1.00	37.24	AAAA
ATOM	11	CA	ARG	A	8	-4.469	3.076	33.906	1.00	34.91	AAAA
ATOM	12	CB	ARG	A	8	-5.782	3.109	34.686	1.00	36.65	AAAA
ATOM	13	CG	ARG	A	8	-5.950	2.017	35.721	1.00	39.89	AAAA
ATOM	14	CD	ARG	A	8	-7.323	2.124	36.356	1.00	42.12	AAAA
ATOM	15	NE	ARG	A	8	-7.663	0.960	37.163	1.00	45.03	AAAA
ATOM	16	CZ	ARG	A	8	-7.031	0.610	38.279	1.00	46.29	AAAA
ATOM	17	NH1	ARG	A	8	-6.015	1.337	38.725	1.00	46.88	AAAA
ATOM	18	NH2	ARG	A	8	-7.420	-0.466	38.952	1.00	47.41	AAAA
ATOM	19	C	ARG	A	8	-4.584	3.999	32.696	1.00	32.27	AAAA
ATOM	20	O	ARG	A	8	-4.602	5.224	32.832	1.00	31.60	AAAA
ATOM	21	N	LEU	A	9	-4.663	3.403	31.512	1.00	29.57	AAAA
ATOM	22	CA	LEU	A	9	-4.792	4.171	30.283	1.00	27.45	AAAA
ATOM	23	CB	LEU	A	9	-3.581	3.954	29.362	1.00	26.31	AAAA
ATOM	24	CG	LEU	A	9	-3.752	4.466	27.916	1.00	25.77	AAAA
ATOM	25	CD1	LEU	A	9	-3.670	5.985	27.895	1.00	24.31	AAAA

```
ATOM     26  CD2 LEU A   9      -2.679   3.870  26.993  1.00 26.22 AAAA
ATOM     27  C   LEU A   9      -6.038   3.752  29.523  1.00 25.97 AAAA
ATOM     28  O   LEU A   9      -6.397   2.587  29.485  1.00 25.57 AAAA
ATOM     29  N   MET A  10      -6.713   4.738  28.928  1.00 25.37 AAAA
ATOM     30  CA  MET A  10      -7.866   4.429  28.101  1.00 24.70 AAAA
ATOM     31  CB  MET A  10      -9.142   5.101  28.612  1.00 25.60 AAAA
ATOM     32  CG  MET A  10     -10.323   4.873  27.675  1.00 25.77 AAAA
ATOM     33  SD  MET A  10     -11.916   4.958  28.492  1.00 26.63 AAAA
ATOM     34  CE  MET A  10     -12.197   3.222  28.862  1.00 25.72 AAAA
ATOM     35  C   MET A  10      -7.528   4.943  26.715  1.00 23.31 AAAA
ATOM     36  O   MET A  10      -7.198   6.116  26.544  1.00 24.02 AAAA
ATOM     37  N   VAL A  11      -7.574   4.059  25.727  1.00 22.25 AAAA
ATOM     38  CA  VAL A  11      -7.278   4.461  24.359  1.00 22.34 AAAA
ATOM     39  CB  VAL A  11      -6.444   3.386  23.624  1.00 22.75 AAAA
ATOM     40  CG1 VAL A  11      -6.256   3.768  22.158  1.00 20.51 AAAA
ATOM     41  CG2 VAL A  11      -5.082   3.239  24.310  1.00 21.75 AAAA
ATOM     42  C   VAL A  11      -8.612   4.654  23.646  1.00 22.94 AAAA
ATOM     43  O   VAL A  11      -9.525   3.843  23.804  1.00 23.37 AAAA
ATOM     44  N   MET A  12      -8.722   5.734  22.878  1.00 22.18 AAAA
ATOM     45  CA  MET A  12      -9.949   6.034  22.146  1.00 23.10 AAAA
ATOM     46  CB  MET A  12     -10.496   7.399  22.589  1.00 22.78 AAAA
ATOM     47  CG  MET A  12     -10.359   7.655  24.096  1.00 23.92 AAAA
ATOM     48  SD  MET A  12     -10.955   9.279  24.657  1.00 25.51 AAAA
ATOM     49  CE  MET A  12      -9.641  10.349  24.162  1.00 22.79 AAAA
ATOM     50  C   MET A  12      -9.582   6.072  20.673  1.00 22.97 AAAA
ATOM     51  O   MET A  12      -8.917   6.997  20.226  1.00 21.16 AAAA
ATOM     52  N   ALA A  13      -9.992   5.057  19.921  1.00 26.97 AAAA
ATOM     53  CA  ALA A  13      -9.665   5.008  18.498  1.00 30.88 AAAA
ATOM     54  CB  ALA A  13      -8.381   4.212  18.288  1.00 31.18 AAAA
ATOM     55  C   ALA A  13     -10.813   4.412  17.685  1.00 34.35 AAAA
ATOM     56  O   ALA A  13     -11.328   3.335  18.006  1.00 35.86 AAAA
ATOM     57  N   GLY A  14     -11.176   5.127  16.622  1.00 37.37 AAAA
ATOM     58  CA  GLY A  14     -12.287   4.762  15.757  1.00 40.54 AAAA
ATOM     59  C   GLY A  14     -12.239   3.583  14.808  1.00 41.52 AAAA
ATOM     60  O   GLY A  14     -11.267   2.831  14.755  1.00 43.26 AAAA
ATOM     61  N   GLY A  15     -13.322   3.451  14.042  1.00 42.70 AAAA
ATOM     62  CA  GLY A  15     -13.491   2.363  13.094  1.00 43.13 AAAA
ATOM     63  C   GLY A  15     -12.660   2.286  11.825  1.00 43.41 AAAA
ATOM     64  O   GLY A  15     -13.212   2.187  10.730  1.00 44.39 AAAA
ATOM     65  N   THR A  16     -11.340   2.333  11.966  1.00 43.38 AAAA
ATOM     66  CA  THR A  16     -10.426   2.204  10.833  1.00 43.22 AAAA
ATOM     67  CB  THR A  16     -10.120   3.551  10.110  1.00 44.23 AAAA
ATOM     68  OG1 THR A  16      -9.302   4.375  10.949  1.00 44.41 AAAA
ATOM     69  CG2 THR A  16     -11.404   4.286   9.754  1.00 43.74 AAAA
ATOM     70  C   THR A  16      -9.118   1.679  11.402  1.00 43.06 AAAA
ATOM     71  O   THR A  16      -8.728   2.042  12.517  1.00 42.99 AAAA
ATOM     72  N   GLY A  17      -8.453   0.810  10.649  1.00 41.81 AAAA
ATOM     73  CA  GLY A  17      -7.190   0.268  11.109  1.00 40.71 AAAA
ATOM     74  C   GLY A  17      -6.202   1.401  11.275  1.00 39.54 AAAA
ATOM     75  O   GLY A  17      -5.275   1.330  12.085  1.00 39.73 AAAA
ATOM     76  N   GLY A  18      -6.413   2.460  10.500  1.00 37.79 AAAA
ATOM     77  CA  GLY A  18      -5.539   3.611  10.572  1.00 35.68 AAAA
ATOM     78  C   GLY A  18      -5.394   4.116  11.994  1.00 34.88 AAAA
ATOM     79  O   GLY A  18      -4.285   4.441  12.427  1.00 35.21 AAAA
ATOM     80  N   HIS A  19      -6.503   4.186  12.728  1.00 32.89 AAAA
ATOM     81  CA  HIS A  19      -6.454   4.664  14.110  1.00 32.14 AAAA
ATOM     82  CB  HIS A  19      -7.759   5.371  14.504  1.00 30.28 AAAA
ATOM     83  CG  HIS A  19      -8.150   6.504  13.605  1.00 28.85 AAAA
ATOM     84  CD2 HIS A  19      -9.336   6.808  13.027  1.00 27.83 AAAA
ATOM     85  ND1 HIS A  19      -7.288   7.524  13.265  1.00 28.68 AAAA
ATOM     86  CE1 HIS A  19      -7.926   8.407  12.517  1.00 28.09 AAAA
ATOM     87  NE2 HIS A  19      -9.170   7.996  12.358  1.00 27.45 AAAA
ATOM     88  C   HIS A  19      -6.229   3.533  15.108  1.00 31.91 AAAA
ATOM     89  O   HIS A  19      -5.480   3.684  16.072  1.00 31.76 AAAA
ATOM     90  N   VAL A  20      -6.895   2.407  14.881  1.00 31.82 AAAA
ATOM     91  CA  VAL A  20      -6.813   1.271  15.788  1.00 33.08 AAAA
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ATOM	94	CG2	VAL	A	20	-9.260	0.830	15.540	1.00	34.25	AAAA
ATOM	95	C	VAL	A	20	-5.452	0.587	15.898	1.00	33.31	AAAA
ATOM	96	O	VAL	A	20	-4.977	0.337	17.008	1.00	32.99	AAAA
ATOM	97	N	PHE	A	21	-4.823	0.288	14.765	1.00	33.64	AAAA
ATOM	98	CA	PHE	A	21	-3.526	-0.385	14.794	1.00	33.68	AAAA
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ATOM	100	CG	PHE	A	21	-3.900	-1.578	12.577	1.00	39.10	AAAA
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ATOM	109	CD	PRO	A	22	-2.939	2.544	14.400	1.00	31.41	AAAA
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ATOM	127	N	ALA	A	25	-0.555	-0.743	19.296	1.00	27.77	AAAA
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ATOM	137	C	VAL	A	26	0.409	1.131	23.450	1.00	29.18	AAAA
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ATOM	150	CE1	HIS	A	28	-1.696	-6.600	22.670	1.00	32.38	AAAA
ATOM	151	NE2	HIS	A	28	-1.747	-6.112	21.443	1.00	32.85	AAAA
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ATOM	208	CZ3	TRP	A	35	-0.563	5.095	31.348	1.00	37.99	AAAA
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ATOM	234	CZ	ARG	A	38	-13.464	-2.495	31.308	1.00	43.12	AAAA
ATOM	235	NH1	ARG	A	38	-12.697	-3.142	32.176	1.00	43.84	AAAA
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ATOM	244	CE2	TRP	A	39	-8.995	0.945	20.661	1.00	34.00	AAAA
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ATOM	262	CA	GLY	A	41	-14.946	2.553	20.821	1.00	25.95	AAAA
ATOM	263	C	GLY	A	41	-16.426	2.332	20.594	1.00	28.01	AAAA
ATOM	264	O	GLY	A	41	-17.234	2.555	21.494	1.00	28.82	AAAA
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ATOM	267	CB	THR	A	42	-18.603	2.497	17.855	1.00	32.12	AAAA
ATOM	268	OG1	THR	A	42	-18.293	3.871	18.119	1.00	34.95	AAAA
ATOM	269	CG2	THR	A	42	-20.098	2.367	17.611	1.00	34.55	AAAA
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ATOM	278	CA	ASP	A	44	-20.557	-1.671	15.361	1.00	42.78	AAAA
ATOM	279	CB	ASP	A	44	-21.678	-0.812	14.774	1.00	44.80	AAAA
ATOM	280	CG	ASP	A	44	-21.438	0.670	14.973	1.00	46.37	AAAA
ATOM	281	OD1	ASP	A	44	-20.464	1.206	14.400	1.00	48.22	AAAA
ATOM	282	OD2	ASP	A	44	-22.220	1.302	15.712	1.00	49.14	AAAA
ATOM	283	C	ASP	A	44	-19.324	-1.559	14.472	1.00	43.14	AAAA
ATOM	284	O	ASP	A	44	-19.320	-2.061	13.349	1.00	44.14	AAAA
ATOM	285	N	ARG	A	45	-18.281	-0.904	14.970	1.00	42.77	AAAA
ATOM	286	CA	ARG	A	45	-17.056	-0.730	14.199	1.00	42.34	AAAA
ATOM	287	CB	ARG	A	45	-16.415	0.614	14.550	1.00	44.43	AAAA
ATOM	288	CG	ARG	A	45	-17.206	1.822	14.056	1.00	48.23	AAAA
ATOM	289	CD	ARG	A	45	-17.272	1.845	12.533	1.00	51.20	AAAA

ATOM	290	NE	ARG	A	45	-17.950	3.029	12.014	1.00	54.35	AAAA
ATOM	291	CZ	ARG	A	45	-17.526	4.270	12.191	1.00	56.26	AAAA
ATOM	292	NH1	ARG	A	45	-16.417	4.522	12.881	1.00	56.45	AAAA
ATOM	293	NH2	ARG	A	45	-18.212	5.290	11.670	1.00	57.50	AAAA
ATOM	294	C	ARG	A	45	-16.054	-1.872	14.401	1.00	41.11	AAAA
ATOM	295	O	ARG	A	45	-16.194	-2.679	15.320	1.00	40.45	AAAA
ATOM	296	N	MET	A	46	-15.041	-1.928	13.543	1.00	39.55	AAAA
ATOM	297	CA	MET	A	46	-14.038	-2.990	13.604	1.00	39.67	AAAA
ATOM	298	CB	MET	A	46	-13.041	-2.839	12.444	1.00	39.68	AAAA
ATOM	299	CG	MET	A	46	-12.239	-1.544	12.423	1.00	42.15	AAAA
ATOM	300	SD	MET	A	46	-10.690	-1.620	13.352	1.00	44.74	AAAA
ATOM	301	CE	MET	A	46	-9.559	-2.332	12.128	1.00	41.92	AAAA
ATOM	302	C	MET	A	46	-13.279	-3.148	14.926	1.00	38.68	AAAA
ATOM	303	O	MET	A	46	-12.772	-4.232	15.219	1.00	38.02	AAAA
ATOM	304	N	GLU	A	47	-13.198	-2.092	15.730	1.00	37.48	AAAA
ATOM	305	CA	GLU	A	47	-12.486	-2.198	17.002	1.00	36.91	AAAA
ATOM	306	CB	GLU	A	47	-12.309	-0.820	17.650	1.00	35.19	AAAA
ATOM	307	CG	GLU	A	47	-13.615	-0.150	18.058	1.00	34.12	AAAA
ATOM	308	CD	GLU	A	47	-14.142	0.807	17.003	1.00	34.06	AAAA
ATOM	309	OE1	GLU	A	47	-13.712	0.707	15.832	1.00	33.13	AAAA
ATOM	310	OE2	GLU	A	47	-14.995	1.652	17.350	1.00	32.08	AAAA
ATOM	311	C	GLU	A	47	-13.225	-3.123	17.972	1.00	36.96	AAAA
ATOM	312	O	GLU	A	47	-12.612	-3.744	18.842	1.00	37.00	AAAA
ATOM	313	N	ALA	A	48	-14.541	-3.222	17.818	1.00	36.76	AAAA
ATOM	314	CA	ALA	A	48	-15.342	-4.066	18.700	1.00	36.98	AAAA
ATOM	315	CB	ALA	A	48	-16.823	-3.917	18.365	1.00	37.33	AAAA
ATOM	316	C	ALA	A	48	-14.943	-5.533	18.623	1.00	38.23	AAAA
ATOM	317	O	ALA	A	48	-15.100	-6.281	19.590	1.00	37.91	AAAA
ATOM	318	N	ASP	A	49	-14.430	-5.947	17.470	1.00	39.31	AAAA
ATOM	319	CA	ASP	A	49	-14.027	-7.332	17.286	1.00	40.97	AAAA
ATOM	320	CB	ASP	A	49	-14.477	-7.832	15.909	1.00	42.68	AAAA
ATOM	321	CG	ASP	A	49	-15.988	-7.912	15.783	1.00	44.91	AAAA
ATOM	322	OD1	ASP	A	49	-16.612	-8.681	16.549	1.00	45.64	AAAA
ATOM	323	OD2	ASP	A	49	-16.552	-7.205	14.918	1.00	46.44	AAAA
ATOM	324	C	ASP	A	49	-12.524	-7.519	17.426	1.00	40.10	AAAA
ATOM	325	O	ASP	A	49	-12.069	-8.518	17.974	1.00	40.92	AAAA
ATOM	326	N	LEU	A	50	-11.761	-6.549	16.940	1.00	39.40	AAAA
ATOM	327	CA	LEU	A	50	-10.306	-6.623	16.982	1.00	39.05	AAAA
ATOM	328	CB	LEU	A	50	-9.710	-5.578	16.036	1.00	38.17	AAAA
ATOM	329	CG	LEU	A	50	-8.183	-5.562	15.942	1.00	38.18	AAAA
ATOM	330	CD1	LEU	A	50	-7.685	-6.916	15.462	1.00	37.91	AAAA
ATOM	331	CD2	LEU	A	50	-7.740	-4.460	14.999	1.00	37.50	AAAA
ATOM	332	C	LEU	A	50	-9.666	-6.486	18.365	1.00	39.12	AAAA
ATOM	333	O	LEU	A	50	-8.805	-7.286	18.732	1.00	38.56	AAAA
ATOM	334	N	VAL	A	51	-10.084	-5.483	19.132	1.00	38.79	AAAA
ATOM	335	CA	VAL	A	51	-9.516	-5.257	20.459	1.00	37.64	AAAA
ATOM	336	CB	VAL	A	51	-10.127	-3.989	21.111	1.00	36.87	AAAA
ATOM	337	CG1	VAL	A	51	-9.571	-3.795	22.523	1.00	35.15	AAAA
ATOM	338	CG2	VAL	A	51	-9.810	-2.777	20.256	1.00	34.42	AAAA
ATOM	339	C	VAL	A	51	-9.647	-6.449	21.415	1.00	37.87	AAAA
ATOM	340	O	VAL	A	51	-8.695	-6.790	22.115	1.00	37.54	AAAA
ATOM	341	N	PRO	A	52	-10.825	-7.093	21.465	1.00	38.44	AAAA
ATOM	342	CD	PRO	A	52	-12.141	-6.700	20.932	1.00	38.92	AAAA
ATOM	343	CA	PRO	A	52	-10.959	-8.237	22.373	1.00	39.32	AAAA
ATOM	344	CB	PRO	A	52	-12.436	-8.602	22.253	1.00	39.97	AAAA
ATOM	345	CG	PRO	A	52	-13.080	-7.277	21.962	1.00	38.98	AAAA
ATOM	346	C	PRO	A	52	-10.035	-9.392	21.974	1.00	40.07	AAAA
ATOM	347	O	PRO	A	52	-9.685	-10.232	22.805	1.00	40.30	AAAA
ATOM	348	N	LYS	A	53	-9.649	-9.427	20.699	1.00	40.35	AAAA
ATOM	349	CA	LYS	A	53	-8.752	-10.463	20.193	1.00	40.58	AAAA
ATOM	350	CB	LYS	A	53	-8.812	-10.541	18.661	1.00	41.25	AAAA
ATOM	351	CG	LYS	A	53	-10.093	-11.169	18.129	1.00	43.24	AAAA
ATOM	352	CD	LYS	A	53	-10.033	-11.383	16.627	1.00	44.40	AAAA
ATOM	353	CE	LYS	A	53	-11.280	-12.102	16.133	1.00	45.87	AAAA
ATOM	354	NZ	LYS	A	53	-11.250	-12.342	14.659	1.00	47.88	AAAA
ATOM	355	C	LYS	A	53	-7.323	-10.184	20.636	1.00	39.99	AAAA

ATOM	356	O	LYS	A	53	-6.426	-11.006	20.432	1.00	39.70	AAAA
ATOM	357	N	HIS	A	54	-7.112	-9.01	21.231	1.00	38.65	AAAA
ATOM	358	CA	HIS	A	54	-5.790	-8.642	21.727	1.00	37.71	AAAA
ATOM	359	CB	HIS	A	54	-5.408	-7.233	21.272	1.00	37.50	AAAA
ATOM	360	CG	HIS	A	54	-4.903	-7.164	19.864	1.00	37.59	AAAA
ATOM	361	CD2	HIS	A	54	-5.483	-7.502	18.687	1.00	37.67	AAAA
ATOM	362	ND1	HIS	A	54	-3.658	-6.666	19.546	1.00	37.90	AAAA
ATOM	363	CE1	HIS	A	54	-3.492	-6.698	18.235	1.00	37.11	AAAA
ATOM	364	NE2	HIS	A	54	-4.586	-7.202	17.691	1.00	36.75	AAAA
ATOM	365	C	HIS	A	54	-5.788	-8.711	23.248	1.00	37.10	AAAA
ATOM	366	O	HIS	A	54	-4.871	-8.214	23.899	1.00	37.35	AAAA
ATOM	367	N	GLY	A	55	-6.828	-9.331	23.800	1.00	36.15	AAAA
ATOM	368	CA	GLY	A	55	-6.948	-9.477	25.240	1.00	36.70	AAAA
ATOM	369	C	GLY	A	55	-7.266	-8.200	25.997	1.00	36.66	AAAA
ATOM	370	O	GLY	A	55	-7.145	-8.157	27.222	1.00	36.89	AAAA
ATOM	371	N	ILE	A	56	-7.686	-7.163	25.277	1.00	35.61	AAAA
ATOM	372	CA	ILE	A	56	-8.009	-5.885	25.900	1.00	34.03	AAAA
ATOM	373	CB	ILE	A	56	-7.389	-4.723	25.100	1.00	32.39	AAAA
ATOM	374	CG2	ILE	A	56	-7.748	-3.386	25.750	1.00	31.80	AAAA
ATOM	375	CG1	ILE	A	56	-5.869	-4.904	25.031	1.00	31.50	AAAA
ATOM	376	CD1	ILE	A	56	-5.149	-3.900	24.144	1.00	30.46	AAAA
ATOM	377	C	ILE	A	56	-9.516	-5.668	26.017	1.00	34.37	AAAA
ATOM	378	O	ILE	A	56	-10.263	-5.908	25.067	1.00	34.29	AAAA
ATOM	379	N	GLU	A	57	-9.955	-5.224	27.193	1.00	34.18	AAAA
ATOM	380	CA	GLU	A	57	-11.370	-4.969	27.432	1.00	34.19	AAAA
ATOM	381	CB	GLU	A	57	-11.638	-4.733	28.922	1.00	37.08	AAAA
ATOM	382	CG	GLU	A	57	-11.301	-5.913	29.837	1.00	41.06	AAAA
ATOM	383	CD	GLU	A	57	-12.180	-7.127	29.591	1.00	44.07	AAAA
ATOM	384	OE1	GLU	A	57	-12.011	-8.135	30.313	1.00	45.83	AAAA
ATOM	385	OE2	GLU	A	57	-13.040	-7.078	28.682	1.00	46.00	AAAA
ATOM	386	C	GLU	A	57	-11.751	-3.723	26.645	1.00	32.88	AAAA
ATOM	387	O	GLU	A	57	-10.905	-2.870	26.368	1.00	31.69	AAAA
ATOM	388	N	ILE	A	58	-13.022	-3.611	26.285	1.00	31.36	AAAA
ATOM	389	CA	ILE	A	58	-13.454	-2.454	25.529	1.00	29.92	AAAA
ATOM	390	CB	ILE	A	58	-13.390	-2.749	24.009	1.00	29.51	AAAA
ATOM	391	CG2	ILE	A	58	-14.175	-4.015	23.689	1.00	28.67	AAAA
ATOM	392	CG1	ILE	A	58	-13.895	-1.543	23.216	1.00	29.61	AAAA
ATOM	393	CD1	ILE	A	58	-13.578	-1.623	21.734	1.00	29.09	AAAA
ATOM	394	C	ILE	A	58	-14.843	-1.984	25.927	1.00	29.49	AAAA
ATOM	395	O	ILE	A	58	-15.791	-2.764	25.968	1.00	27.83	AAAA
ATOM	396	N	ASP	A	59	-14.939	-0.700	26.252	1.00	29.28	AAAA
ATOM	397	CA	ASP	A	59	-16.202	-0.091	26.626	1.00	29.70	AAAA
ATOM	398	CB	ASP	A	59	-15.999	0.916	27.759	1.00	30.90	AAAA
ATOM	399	CG	ASP	A	59	-15.676	0.245	29.083	1.00	32.17	AAAA
ATOM	400	OD1	ASP	A	59	-16.485	-0.591	29.540	1.00	33.00	AAAA
ATOM	401	OD2	ASP	A	59	-14.615	0.554	29.664	1.00	33.03	AAAA
ATOM	402	C	ASP	A	59	-16.723	0.608	25.378	1.00	30.39	AAAA
ATOM	403	O	ASP	A	59	-15.947	1.165	24.600	1.00	30.45	AAAA
ATOM	404	N	PHE	A	60	-18.033	0.570	25.180	1.00	31.29	AAAA
ATOM	405	CA	PHE	A	60	-18.612	1.183	24.000	1.00	32.36	AAAA
ATOM	406	CB	PHE	A	60	-19.469	0.166	23.239	1.00	33.01	AAAA
ATOM	407	CG	PHE	A	60	-18.720	-1.056	22.793	1.00	33.55	AAAA
ATOM	408	CD1	PHE	A	60	-19.033	-2.307	23.318	1.00	34.07	AAAA
ATOM	409	CD2	PHE	A	60	-17.720	-0.964	21.832	1.00	34.02	AAAA
ATOM	410	CE1	PHE	A	60	-18.362	-3.451	22.890	1.00	33.73	AAAA
ATOM	411	CE2	PHE	A	60	-17.042	-2.104	21.397	1.00	34.93	AAAA
ATOM	412	CZ	PHE	A	60	-17.366	-3.348	21.928	1.00	34.12	AAAA
ATOM	413	C	PHE	A	60	-19.469	2.395	24.300	1.00	32.89	AAAA
ATOM	414	O	PHE	A	60	-20.062	2.508	25.372	1.00	33.13	AAAA
ATOM	415	N	ILE	A	61	-19.502	3.309	23.338	1.00	34.43	AAAA
ATOM	416	CA	ILE	A	61	-20.326	4.500	23.421	1.00	36.08	AAAA
ATOM	417	CB	ILE	A	61	-19.545	5.785	23.056	1.00	36.15	AAAA
ATOM	418	CG2	ILE	A	61	-20.511	6.957	22.913	1.00	36.47	AAAA
ATOM	419	CG1	ILE	A	61	-18.504	6.092	24.136	1.00	37.27	AAAA
ATOM	420	CD1	ILE	A	61	-17.711	7.360	23.875	1.00	38.32	AAAA
ATOM	421	C	ILE	A	61	-21.380	4.230	22.353	1.00	37.27	AAAA

ATOM	422	O	ILE	A	61	-21.050	3.901	21.215	1.00	36.29	AAAA
ATOM	423	N	ARG	A	62	-22.644	4.337	22.728	1.00	39.91	AAAA
ATOM	424	CA	ARG	A	62	-23.732	4.087	21.797	1.00	43.16	AAAA
ATOM	425	CB	ARG	A	62	-24.818	3.268	22.494	1.00	44.19	AAAA
ATOM	426	CG	ARG	A	62	-26.183	3.312	21.825	1.00	48.33	AAAA
ATOM	427	CD	ARG	A	62	-27.207	2.581	22.680	1.00	50.28	AAAA
ATOM	428	NE	ARG	A	62	-28.584	2.906	22.319	1.00	52.71	AAAA
ATOM	429	CZ	ARG	A	62	-29.646	2.419	22.951	1.00	53.14	AAAA
ATOM	430	NH1	ARG	A	62	-29.482	1.586	23.968	1.00	54.03	AAAA
ATOM	431	NH2	ARG	A	62	-30.870	2.767	22.573	1.00	53.49	AAAA
ATOM	432	C	ARG	A	62	-24.302	5.400	21.280	1.00	44.33	AAAA
ATOM	433	O	ARG	A	62	-24.942	6.140	22.021	1.00	43.98	AAAA
ATOM	434	N	ILE	A	63	-24.053	5.686	20.005	1.00	46.60	AAAA
ATOM	435	CA	ILE	A	63	-24.537	6.912	19.378	1.00	49.26	AAAA
ATOM	436	CB	ILE	A	63	-23.369	7.834	18.965	1.00	49.17	AAAA
ATOM	437	CG2	ILE	A	63	-23.903	9.208	18.593	1.00	50.31	AAAA
ATOM	438	CG1	ILE	A	63	-22.368	7.967	20.113	1.00	49.48	AAAA
ATOM	439	CD1	ILE	A	63	-21.158	8.822	19.775	1.00	49.03	AAAA
ATOM	440	C	ILE	A	63	-25.316	6.540	18.123	1.00	50.72	AAAA
ATOM	441	O	ILE	A	63	-24.724	6.219	17.093	1.00	50.90	AAAA
ATOM	442	N	SER	A	64	-26.639	6.591	18.209	1.00	52.58	AAAA
ATOM	443	CA	SER	A	64	-27.488	6.235	17.078	1.00	54.45	AAAA
ATOM	444	CB	SER	A	64	-28.731	5.491	17.574	1.00	54.65	AAAA
ATOM	445	OG	SER	A	64	-29.528	6.329	18.391	1.00	55.29	AAAA
ATOM	446	C	SER	A	64	-27.927	7.433	16.242	1.00	55.33	AAAA
ATOM	447	O	SER	A	64	-27.919	8.571	16.713	1.00	55.34	AAAA
ATOM	448	N	GLY	A	65	-28.301	7.158	14.993	1.00	56.31	AAAA
ATOM	449	CA	GLY	A	65	-28.774	8.196	14.090	1.00	57.42	AAAA
ATOM	450	C	GLY	A	65	-27.751	9.156	13.508	1.00	58.34	AAAA
ATOM	451	O	GLY	A	65	-28.052	10.333	13.315	1.00	58.53	AAAA
ATOM	452	N	LEU	A	66	-26.552	8.668	13.207	1.00	59.08	AAAA
ATOM	453	CA	LEU	A	66	-25.514	9.530	12.648	1.00	59.80	AAAA
ATOM	454	CB	LEU	A	66	-24.147	9.153	13.229	1.00	59.99	AAAA
ATOM	455	CG	LEU	A	66	-23.927	9.513	14.704	1.00	60.38	AAAA
ATOM	456	CD1	LEU	A	66	-23.983	11.026	14.877	1.00	60.37	AAAA
ATOM	457	CD2	LEU	A	66	-24.983	8.840	15.565	1.00	60.47	AAAA
ATOM	458	C	LEU	A	66	-25.467	9.497	11.121	1.00	60.04	AAAA
ATOM	459	O	LEU	A	66	-25.049	10.466	10.484	1.00	59.29	AAAA
ATOM	460	N	ARG	A	67	-25.892	8.378	10.541	1.00	60.97	AAAA
ATOM	461	CA	ARG	A	67	-25.923	8.224	9.089	1.00	61.57	AAAA
ATOM	462	CB	ARG	A	67	-26.860	9.273	8.484	1.00	62.96	AAAA
ATOM	463	CG	ARG	A	67	-28.340	8.984	8.698	1.00	65.29	AAAA
ATOM	464	CD	ARG	A	67	-29.138	10.270	8.842	1.00	66.93	AAAA
ATOM	465	NE	ARG	A	67	-30.566	10.067	8.611	1.00	68.58	AAAA
ATOM	466	CZ	ARG	A	67	-31.514	10.924	8.980	1.00	69.56	AAAA
ATOM	467	NH1	ARG	A	67	-31.192	12.048	9.607	1.00	69.39	AAAA
ATOM	468	NH2	ARG	A	67	-32.788	10.665	8.709	1.00	69.97	AAAA
ATOM	469	C	ARG	A	67	-24.558	8.301	8.409	1.00	61.08	AAAA
ATOM	470	O	ARG	A	67	-24.474	8.448	7.191	1.00	61.57	AAAA
ATOM	471	N	GLY	A	68	-23.489	8.204	9.189	1.00	60.22	AAAA
ATOM	472	CA	GLY	A	68	-22.161	8.249	8.605	1.00	58.95	AAAA
ATOM	473	C	GLY	A	68	-21.531	9.627	8.541	1.00	58.19	AAAA
ATOM	474	O	GLY	A	68	-20.373	9.763	8.140	1.00	58.31	AAAA
ATOM	475	N	LYS	A	69	-22.282	10.655	8.921	1.00	57.03	AAAA
ATOM	476	CA	LYS	A	69	-21.746	12.009	8.904	1.00	55.91	AAAA
ATOM	477	CB	LYS	A	69	-22.812	13.015	9.349	1.00	56.90	AAAA
ATOM	478	CG	LYS	A	69	-23.827	13.368	8.264	1.00	57.91	AAAA
ATOM	479	CD	LYS	A	69	-23.167	14.147	7.133	1.00	58.56	AAAA
ATOM	480	CE	LYS	A	69	-24.163	14.517	6.044	1.00	59.37	AAAA
ATOM	481	NZ	LYS	A	69	-23.522	15.327	4.965	1.00	59.41	AAAA
ATOM	482	C	LYS	A	69	-20.527	12.078	9.818	1.00	54.19	AAAA
ATOM	483	O	LYS	A	69	-19.447	12.480	9.392	1.00	54.69	AAAA
ATOM	484	N	GLY	A	70	-20.697	11.676	11.072	1.00	51.77	AAAA
ATOM	485	CA	GLY	A	70	-19.575	11.692	11.991	1.00	48.95	AAAA
ATOM	486	C	GLY	A	70	-19.668	12.687	13.129	1.00	46.84	AAAA
ATOM	487	O	GLY	A	70	-20.754	12.975	13.629	1.00	46.29	AAAA

ATOM	488	N	ILE	A	71	-18.515	13.221	13.523	1.00	45.26	AAAA
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ATOM	714	O	ASP	A	98	-4.267	10.486	33.681	1.00	22.57	AAAA
ATOM	715	N	VAL	A	99	-4.918	8.807	32.339	1.00	24.10	AAAA
ATOM	716	CA	VAL	A	99	-4.740	9.569	31.111	1.00	23.85	AAAA
ATOM	717	CB	VAL	A	99	-3.237	9.633	30.730	1.00	25.11	AAAA
ATOM	718	CG1	VAL	A	99	-2.684	8.220	30.614	1.00	25.72	AAAA
ATOM	719	CG2	VAL	A	99	-3.044	10.372	29.420	1.00	24.76	AAAA
ATOM	720	C	VAL	A	99	-5.498	8.865	29.989	1.00	22.90	AAAA
ATOM	721	O	VAL	A	99	-5.767	7.667	30.073	1.00	22.05	AAAA
ATOM	722	N	VAL	A	100	-5.869	9.613	28.951	1.00	22.07	AAAA
ATOM	723	CA	VAL	A	100	-6.544	9.008	27.808	1.00	21.38	AAAA
ATOM	724	CB	VAL	A	100	-8.038	9.451	27.663	1.00	21.17	AAAA
ATOM	725	CG1	VAL	A	100	-8.804	9.095	28.914	1.00	21.06	AAAA
ATOM	726	CG2	VAL	A	100	-8.139	10.942	27.354	1.00	22.14	AAAA
ATOM	727	C	VAL	A	100	-5.777	9.398	26.559	1.00	21.31	AAAA
ATOM	728	O	VAL	A	100	-5.244	10.505	26.464	1.00	21.01	AAAA
ATOM	729	N	LEU	A	101	-5.701	8.468	25.612	1.00	21.54	AAAA
ATOM	730	CA	LEU	A	101	-4.994	8.697	24.362	1.00	22.01	AAAA
ATOM	731	CB	LEU	A	101	-3.944	7.599	24.139	1.00	23.42	AAAA
ATOM	732	CG	LEU	A	101	-2.691	7.856	23.288	1.00	25.21	AAAA
ATOM	733	CD1	LEU	A	101	-2.230	6.515	22.696	1.00	25.87	AAAA
ATOM	734	CD2	LEU	A	101	-2.930	8.854	22.187	1.00	26.43	AAAA
ATOM	735	C	LEU	A	101	-6.006	8.644	23.222	1.00	21.51	AAAA
ATOM	736	O	LEU	A	101	-6.667	7.625	23.029	1.00	21.94	AAAA
ATOM	737	N	GLY	A	102	-6.127	9.742	22.484	1.00	21.18	AAAA
ATOM	738	CA	GLY	A	102	-7.043	9.780	21.358	1.00	21.84	AAAA
ATOM	739	C	GLY	A	102	-6.246	9.586	20.079	1.00	21.20	AAAA
ATOM	740	O	GLY	A	102	-5.294	10.324	19.837	1.00	22.62	AAAA
ATOM	741	N	MET	A	103	-6.627	8.599	19.270	1.00	21.18	AAAA
ATOM	742	CA	MET	A	103	-5.933	8.312	18.015	1.00	22.83	AAAA
ATOM	743	CB	MET	A	103	-5.715	6.805	17.865	1.00	23.16	AAAA
ATOM	744	CG	MET	A	103	-4.978	6.140	19.030	1.00	24.31	AAAA
ATOM	745	SD	MET	A	103	-3.333	6.804	19.308	1.00	27.62	AAAA
ATOM	746	CE	MET	A	103	-2.455	6.156	17.873	1.00	26.43	AAAA
ATOM	747	C	MET	A	103	-6.709	8.823	16.795	1.00	23.47	AAAA
ATOM	748	O	MET	A	103	-6.351	8.532	15.653	1.00	23.75	AAAA
ATOM	749	N	GLY	A	104	-7.767	9.590	17.043	1.00	25.38	AAAA
ATOM	750	CA	GLY	A	104	-8.585	10.114	15.959	1.00	25.56	AAAA
ATOM	751	C	GLY	A	104	-9.878	9.326	15.833	1.00	25.55	AAAA
ATOM	752	O	GLY	A	104	-10.004	8.241	16.404	1.00	26.58	AAAA
ATOM	753	N	GLY	A	105	-10.840	9.854	15.082	1.00	26.06	AAAA
ATOM	754	CA	GLY	A	105	-12.107	9.159	14.930	1.00	26.21	AAAA
ATOM	755	C	GLY	A	105	-13.140	9.819	15.823	1.00	26.96	AAAA
ATOM	756	O	GLY	A	105	-12.810	10.258	16.926	1.00	25.49	AAAA
ATOM	757	N	TYR	A	106	-14.393	9.863	15.376	1.00	27.65	AAAA
ATOM	758	CA	TYR	A	106	-15.434	10.534	16.145	1.00	28.10	AAAA
ATOM	759	CB	TYR	A	106	-16.759	10.556	15.362	1.00	31.05	AAAA
ATOM	760	CG	TYR	A	106	-17.536	9.257	15.303	1.00	33.49	AAAA
ATOM	761	CD1	TYR	A	106	-18.269	8.802	16.400	1.00	34.81	AAAA

ATOM	762	CE1	TYR	A	106	-19.038	7.634	16.323	1.00	36.18	AAAA
ATOM	763	CD2	TYR	A	106	-17.581	8.509	14.123	1.00	35.64	AAAA
ATOM	764	CE2	TYR	A	106	-18.343	7.344	14.032	1.00	36.47	AAAA
ATOM	765	CZ	TYR	A	106	-19.069	6.912	15.133	1.00	37.27	AAAA
ATOM	766	OH	TYR	A	106	-19.829	5.766	15.027	1.00	38.99	AAAA
ATOM	767	C	TYR	A	106	-15.678	10.072	17.576	1.00	26.46	AAAA
ATOM	768	O	TYR	A	106	-15.976	10.897	18.430	1.00	26.55	AAAA
ATOM	769	N	VAL	A	107	-15.549	8.780	17.858	1.00	25.31	AAAA
ATOM	770	CA	VAL	A	107	-15.783	8.318	19.223	1.00	23.91	AAAA
ATOM	771	CB	VAL	A	107	-15.659	6.772	19.335	1.00	25.47	AAAA
ATOM	772	CG1	VAL	A	107	-14.224	6.327	19.076	1.00	26.57	AAAA
ATOM	773	CG2	VAL	A	107	-16.126	6.315	20.711	1.00	24.96	AAAA
ATOM	774	C	VAL	A	107	-14.836	8.993	20.223	1.00	23.22	AAAA
ATOM	775	O	VAL	A	107	-15.190	9.190	21.389	1.00	23.17	AAAA
ATOM	776	N	SER	A	108	-13.650	9.381	19.765	1.00	23.13	AAAA
ATOM	777	CA	SER	A	108	-12.676	10.029	20.643	1.00	23.40	AAAA
ATOM	778	CB	SER	A	108	-11.301	10.108	19.967	1.00	23.85	AAAA
ATOM	779	OG	SER	A	108	-11.292	11.038	18.899	1.00	25.04	AAAA
ATOM	780	C	SER	A	108	-13.121	11.430	21.044	1.00	23.03	AAAA
ATOM	781	O	SER	A	108	-12.592	12.009	21.993	1.00	22.32	AAAA
ATOM	782	N	GLY	A	109	-14.089	11.979	20.310	1.00	21.84	AAAA
ATOM	783	CA	GLY	A	109	-14.583	13.307	20.627	1.00	21.98	AAAA
ATOM	784	C	GLY	A	109	-15.297	13.342	21.972	1.00	20.30	AAAA
ATOM	785	O	GLY	A	109	-14.898	14.088	22.856	1.00	21.37	AAAA
ATOM	786	N	PRO	A	110	-16.369	12.557	22.155	1.00	20.07	AAAA
ATOM	787	CD	PRO	A	110	-16.992	11.637	21.191	1.00	20.80	AAAA
ATOM	788	CA	PRO	A	110	-17.085	12.550	23.436	1.00	19.58	AAAA
ATOM	789	CB	PRO	A	110	-18.232	11.569	23.199	1.00	20.85	AAAA
ATOM	790	CG	PRO	A	110	-18.398	11.548	21.702	1.00	22.43	AAAA
ATOM	791	C	PRO	A	110	-16.136	12.031	24.524	1.00	18.52	AAAA
ATOM	792	O	PRO	A	110	-16.184	12.462	25.675	1.00	19.12	AAAA
ATOM	793	N	GLY	A	111	-15.286	11.086	24.140	1.00	19.12	AAAA
ATOM	794	CA	GLY	A	111	-14.332	10.525	25.087	1.00	18.87	AAAA
ATOM	795	C	GLY	A	111	-13.402	11.601	25.612	1.00	17.97	AAAA
ATOM	796	O	GLY	A	111	-13.208	11.730	26.813	1.00	19.32	AAAA
ATOM	797	N	GLY	A	112	-12.822	12.380	24.704	1.00	18.62	AAAA
ATOM	798	CA	GLY	A	112	-11.925	13.451	25.105	1.00	17.38	AAAA
ATOM	799	C	GLY	A	112	-12.610	14.509	25.957	1.00	17.36	AAAA
ATOM	800	O	GLY	A	112	-12.035	14.997	26.936	1.00	16.49	AAAA
ATOM	801	N	LEU	A	113	-13.837	14.864	25.583	1.00	16.45	AAAA
ATOM	802	CA	LEU	A	113	-14.611	15.866	26.314	1.00	17.35	AAAA
ATOM	803	CB	LEU	A	113	-15.974	16.079	25.640	1.00	17.68	AAAA
ATOM	804	CG	LEU	A	113	-16.735	17.409	25.805	1.00	21.99	AAAA
ATOM	805	CD1	LEU	A	113	-18.205	17.154	25.511	1.00	20.80	AAAA
ATOM	806	CD2	LEU	A	113	-16.570	18.007	27.178	1.00	22.94	AAAA
ATOM	807	C	LEU	A	113	-14.836	15.329	27.725	1.00	16.05	AAAA
ATOM	808	O	LEU	A	113	-14.695	16.045	28.711	1.00	16.63	AAAA
ATOM	809	N	ALA	A	114	-15.199	14.056	27.801	1.00	16.59	AAAA
ATOM	810	CA	ALA	A	114	-15.442	13.416	29.087	1.00	15.95	AAAA
ATOM	811	CB	ALA	A	114	-15.859	11.963	28.868	1.00	17.72	AAAA
ATOM	812	C	ALA	A	114	-14.194	13.492	29.968	1.00	15.37	AAAA
ATOM	813	O	ALA	A	114	-14.260	13.952	31.105	1.00	15.94	AAAA
ATOM	814	N	ALA	A	115	-13.053	13.050	29.452	1.00	16.63	AAAA
ATOM	815	CA	ALA	A	115	-11.820	13.098	30.251	1.00	15.65	AAAA
ATOM	816	CB	ALA	A	115	-10.641	12.518	29.450	1.00	15.52	AAAA
ATOM	817	C	ALA	A	115	-11.506	14.530	30.693	1.00	16.10	AAAA
ATOM	818	O	ALA	A	115	-11.141	14.777	31.841	1.00	15.67	AAAA
ATOM	819	N	TRP	A	116	-11.650	15.480	29.778	1.00	16.71	AAAA
ATOM	820	CA	TRP	A	116	-11.380	16.873	30.100	1.00	17.31	AAAA
ATOM	821	CB	TRP	A	116	-11.542	17.723	28.835	1.00	18.91	AAAA
ATOM	822	CG	TRP	A	116	-11.172	19.155	29.003	1.00	21.69	AAAA
ATOM	823	CD2	TRP	A	116	-12.008	20.277	28.740	1.00	23.65	AAAA
ATOM	824	CE2	TRP	A	116	-11.262	21.438	29.048	1.00	25.14	AAAA
ATOM	825	CE3	TRP	A	116	-13.321	20.418	28.268	1.00	26.49	AAAA
ATOM	826	CD1	TRP	A	116	-9.979	19.658	29.447	1.00	23.00	AAAA
ATOM	827	NE1	TRP	A	116	-10.025	21.032	29.479	1.00	24.96	AAAA

ATOM	828	CZ2	TRP	A	116	-11.785	22.724	28.902	1.00	26.16	AAAA
ATOM	829	CZ3	TRP	A	116	-13.842	21.702	28.122	1.00	26.44	AAAA
ATOM	830	CH2	TRP	A	116	-13.072	22.834	28.439	1.00	25.35	AAAA
ATOM	831	C	TRP	A	116	-12.292	17.377	31.233	1.00	16.50	AAAA
ATOM	832	O	TRP	A	116	-11.835	18.080	32.137	1.00	16.03	AAAA
ATOM	833	N	SER	A	117	-13.565	16.990	31.200	1.00	16.73	AAAA
ATOM	834	CA	SER	A	117	-14.528	17.399	32.229	1.00	17.06	AAAA
ATOM	835	CB	SER	A	117	-15.961	17.116	31.762	1.00	16.18	AAAA
ATOM	836	OG	SER	A	117	-16.270	15.731	31.743	1.00	18.31	AAAA
ATOM	837	C	SER	A	117	-14.289	16.720	33.586	1.00	18.05	AAAA
ATOM	838	O	SER	A	117	-14.837	17.147	34.605	1.00	17.79	AAAA
ATOM	839	N	LEU	A	118	-13.466	15.678	33.594	1.00	18.13	AAAA
ATOM	840	CA	LEU	A	118	-13.146	14.950	34.827	1.00	19.26	AAAA
ATOM	841	CB	LEU	A	118	-13.262	13.441	34.587	1.00	18.09	AAAA
ATOM	842	CG	LEU	A	118	-14.686	12.932	34.353	1.00	20.04	AAAA
ATOM	843	CD1	LEU	A	118	-14.659	11.484	33.869	1.00	20.30	AAAA
ATOM	844	CD2	LEU	A	118	-15.480	13.064	35.646	1.00	20.40	AAAA
ATOM	845	C	LEU	A	118	-11.736	15.283	35.305	1.00	20.78	AAAA
ATOM	846	O	LEU	A	118	-11.267	14.763	36.321	1.00	20.64	AAAA
ATOM	847	N	GLY	A	119	-11.057	16.152	34.566	1.00	21.27	AAAA
ATOM	848	CA	GLY	A	119	-9.706	16.537	34.943	1.00	21.97	AAAA
ATOM	849	C	GLY	A	119	-8.648	15.519	34.550	1.00	21.55	AAAA
ATOM	850	O	GLY	A	119	-7.515	15.582	35.034	1.00	21.92	AAAA
ATOM	851	N	ILE	A	120	-9.009	14.584	33.678	1.00	20.43	AAAA
ATOM	852	CA	ILE	A	120	-8.082	13.548	33.214	1.00	21.09	AAAA
ATOM	853	CB	ILE	A	120	-8.853	12.270	32.836	1.00	20.95	AAAA
ATOM	854	CG2	ILE	A	120	-7.902	11.226	32.275	1.00	22.20	AAAA
ATOM	855	CG1	ILE	A	120	-9.624	11.748	34.051	1.00	22.05	AAAA
ATOM	856	CD1	ILE	A	120	-10.688	10.709	33.689	1.00	21.95	AAAA
ATOM	857	C	ILE	A	120	-7.358	14.088	31.978	1.00	20.81	AAAA
ATOM	858	O	ILE	A	120	-8.001	14.465	31.004	1.00	21.35	AAAA
ATOM	859	N	PRO	A	121	-6.013	14.131	31.999	1.00	20.67	AAAA
ATOM	860	CD	PRO	A	121	-5.052	13.722	33.040	1.00	20.88	AAAA
ATOM	861	CA	PRO	A	121	-5.320	14.658	30.819	1.00	20.52	AAAA
ATOM	862	CB	PRO	A	121	-3.842	14.649	31.237	1.00	21.37	AAAA
ATOM	863	CG	PRO	A	121	-3.777	13.532	32.240	1.00	22.04	AAAA
ATOM	864	C	PRO	A	121	-5.580	13.893	29.536	1.00	19.38	AAAA
ATOM	865	O	PRO	A	121	-5.717	12.671	29.538	1.00	18.17	AAAA
ATOM	866	N	VAL	A	122	-5.647	14.645	28.442	1.00	20.01	AAAA
ATOM	867	CA	VAL	A	122	-5.903	14.102	27.120	1.00	19.76	AAAA
ATOM	868	CB	VAL	A	122	-7.047	14.866	26.421	1.00	18.63	AAAA
ATOM	869	CG1	VAL	A	122	-7.286	14.281	25.033	1.00	20.46	AAAA
ATOM	870	CG2	VAL	A	122	-8.320	14.790	27.264	1.00	20.31	AAAA
ATOM	871	C	VAL	A	122	-4.672	14.205	26.223	1.00	19.39	AAAA
ATOM	872	O	VAL	A	122	-4.096	15.282	26.069	1.00	19.66	AAAA
ATOM	873	N	VAL	A	123	-4.284	13.079	25.634	1.00	19.86	AAAA
ATOM	874	CA	VAL	A	123	-3.134	13.029	24.734	1.00	20.22	AAAA
ATOM	875	CB	VAL	A	123	-2.086	11.982	25.200	1.00	20.59	AAAA
ATOM	876	CG1	VAL	A	123	-0.898	11.957	24.226	1.00	20.51	AAAA
ATOM	877	CG2	VAL	A	123	-1.602	12.317	26.606	1.00	17.21	AAAA
ATOM	878	C	VAL	A	123	-3.684	12.600	23.381	1.00	21.06	AAAA
ATOM	879	O	VAL	A	123	-4.482	11.666	23.300	1.00	22.10	AAAA
ATOM	880	N	LEU	A	124	-3.269	13.284	22.325	1.00	21.08	AAAA
ATOM	881	CA	LEU	A	124	-3.746	12.952	20.989	1.00	21.68	AAAA
ATOM	882	CB	LEU	A	124	-4.463	14.149	20.366	1.00	21.81	AAAA
ATOM	883	CG	LEU	A	124	-5.629	14.805	21.105	1.00	21.93	AAAA
ATOM	884	CD1	LEU	A	124	-6.133	15.980	20.268	1.00	22.15	AAAA
ATOM	885	CD2	LEU	A	124	-6.737	13.787	21.337	1.00	21.49	AAAA
ATOM	886	C	LEU	A	124	-2.628	12.558	20.038	1.00	21.67	AAAA
ATOM	887	O	LEU	A	124	-1.493	13.011	20.170	1.00	22.39	AAAA
ATOM	888	N	HIS	A	125	-2.964	11.713	19.075	1.00	22.63	AAAA
ATOM	889	CA	HIS	A	125	-2.014	11.336	18.036	1.00	24.74	AAAA
ATOM	890	CB	HIS	A	125	-1.429	9.939	18.244	1.00	24.62	AAAA
ATOM	891	CG	HIS	A	125	-0.471	9.540	17.162	1.00	27.30	AAAA
ATOM	892	CD2	HIS	A	125	-0.629	8.744	16.079	1.00	27.23	AAAA
ATOM	893	ND1	HIS	A	125	0.806	10.057	17.072	1.00	29.96	AAAA

ATOM	894	CE1	HIS	A	125	1.391	9.597	15.979	1.00	27.40	AAAA
ATOM	895	NE2	HIS	A	125	0.541	8.799	15.358	1.00	28.94	AAAA
ATOM	896	C	HIS	A	125	-2.763	11.364	16.705	1.00	24.38	AAAA
ATOM	897	O	HIS	A	125	-3.813	10.741	16.565	1.00	23.93	AAAA
ATOM	898	N	GLU	A	126	-2.233	12.111	15.744	1.00	24.36	AAAA
ATOM	899	CA	GLU	A	126	-2.836	12.199	14.420	1.00	26.31	AAAA
ATOM	900	CB	GLU	A	126	-2.992	13.664	14.005	1.00	25.81	AAAA
ATOM	901	CG	GLU	A	126	-3.465	13.861	12.567	1.00	26.62	AAAA
ATOM	902	CD	GLU	A	126	-4.795	13.196	12.288	1.00	27.69	AAAA
ATOM	903	OE1	GLU	A	126	-5.785	13.544	12.965	1.00	27.90	AAAA
ATOM	904	OE2	GLU	A	126	-4.855	12.326	11.391	1.00	27.53	AAAA
ATOM	905	C	GLU	A	126	-1.901	11.472	13.456	1.00	27.49	AAAA
ATOM	906	O	GLU	A	126	-0.727	11.819	13.349	1.00	27.87	AAAA
ATOM	907	N	GLN	A	127	-2.423	10.463	12.765	1.00	28.80	AAAA
ATOM	908	CA	GLN	A	127	-1.617	9.682	11.834	1.00	30.09	AAAA
ATOM	909	CB	GLN	A	127	-2.192	8.264	11.688	1.00	28.89	AAAA
ATOM	910	CG	GLN	A	127	-2.184	7.421	12.958	1.00	28.94	AAAA
ATOM	911	CD	GLN	A	127	-3.456	7.578	13.775	1.00	29.34	AAAA
ATOM	912	OE1	GLN	A	127	-4.543	7.207	13.329	1.00	29.36	AAAA
ATOM	913	NE2	GLN	A	127	-3.326	8.131	14.973	1.00	28.70	AAAA
ATOM	914	C	GLN	A	127	-1.455	10.277	10.438	1.00	30.92	AAAA
ATOM	915	O	GLN	A	127	-0.428	10.068	9.794	1.00	31.21	AAAA
ATOM	916	N	ASN	A	128	-2.448	11.038	9.986	1.00	32.48	AAAA
ATOM	917	CA	ASN	A	128	-2.434	11.596	8.634	1.00	33.12	AAAA
ATOM	918	CB	ASN	A	128	-3.864	11.589	8.083	1.00	32.20	AAAA
ATOM	919	CG	ASN	A	128	-4.606	10.312	8.424	1.00	33.05	AAAA
ATOM	920	OD1	ASN	A	128	-5.296	10.236	9.445	1.00	33.34	AAAA
ATOM	921	ND2	ASN	A	128	-4.454	9.292	7.584	1.00	31.22	AAAA
ATOM	922	C	ASN	A	128	-1.809	12.971	8.394	1.00	33.60	AAAA
ATOM	923	O	ASN	A	128	-1.571	13.744	9.327	1.00	34.03	AAAA
ATOM	924	N	GLY	A	129	-1.550	13.256	7.117	1.00	33.69	AAAA
ATOM	925	CA	GLY	A	129	-0.959	14.524	6.718	1.00	33.68	AAAA
ATOM	926	C	GLY	A	129	-1.903	15.682	6.972	1.00	33.41	AAAA
ATOM	927	O	GLY	A	129	-1.482	16.834	7.057	1.00	32.92	AAAA
ATOM	928	N	ILE	A	130	-3.192	15.374	7.070	1.00	33.49	AAAA
ATOM	929	CA	ILE	A	130	-4.205	16.383	7.361	1.00	33.06	AAAA
ATOM	930	CB	ILE	A	130	-5.204	16.570	6.206	1.00	33.49	AAAA
ATOM	931	CG2	ILE	A	130	-4.548	17.358	5.083	1.00	35.66	AAAA
ATOM	932	CG1	ILE	A	130	-5.736	15.209	5.751	1.00	34.45	AAAA
ATOM	933	CD1	ILE	A	130	-6.775	15.279	4.665	1.00	35.68	AAAA
ATOM	934	C	ILE	A	130	-4.964	15.892	8.584	1.00	32.19	AAAA
ATOM	935	O	ILE	A	130	-5.379	14.733	8.644	1.00	32.07	AAAA
ATOM	936	N	ALA	A	131	-5.135	16.771	9.561	1.00	31.26	AAAA
ATOM	937	CA	ALA	A	131	-5.832	16.404	10.788	1.00	30.63	AAAA
ATOM	938	CB	ALA	A	131	-5.735	17.547	11.800	1.00	30.70	AAAA
ATOM	939	C	ALA	A	131	-7.292	16.038	10.556	1.00	30.27	AAAA
ATOM	940	O	ALA	A	131	-7.992	16.682	9.774	1.00	30.54	AAAA
ATOM	941	N	GLY	A	132	-7.743	14.987	11.232	1.00	29.03	AAAA
ATOM	942	CA	GLY	A	132	-9.131	14.587	11.119	1.00	27.98	AAAA
ATOM	943	C	GLY	A	132	-9.902	15.678	11.837	1.00	26.80	AAAA
ATOM	944	O	GLY	A	132	-9.326	16.387	12.660	1.00	25.68	AAAA
ATOM	945	N	LEU	A	133	-11.188	15.827	11.543	1.00	26.51	AAAA
ATOM	946	CA	LEU	A	133	-11.973	16.882	12.186	1.00	26.70	AAAA
ATOM	947	CB	LEU	A	133	-13.363	16.967	11.538	1.00	28.16	AAAA
ATOM	948	CG	LEU	A	133	-14.275	18.138	11.936	1.00	28.52	AAAA
ATOM	949	CD1	LEU	A	133	-14.889	17.874	13.280	1.00	32.18	AAAA
ATOM	950	CD2	LEU	A	133	-13.486	19.436	11.960	1.00	30.27	AAAA
ATOM	951	C	LEU	A	133	-12.097	16.713	13.703	1.00	25.88	AAAA
ATOM	952	O	LEU	A	133	-12.063	17.700	14.444	1.00	26.12	AAAA
ATOM	953	N	THR	A	134	-12.240	15.475	14.169	1.00	24.18	AAAA
ATOM	954	CA	THR	A	134	-12.353	15.230	15.608	1.00	23.78	AAAA
ATOM	955	CB	THR	A	134	-12.605	13.729	15.922	1.00	23.18	AAAA
ATOM	956	OG1	THR	A	134	-13.814	13.300	15.285	1.00	23.74	AAAA
ATOM	957	CG2	THR	A	134	-12.751	13.511	17.433	1.00	23.66	AAAA
ATOM	958	C	THR	A	134	-11.071	15.671	16.315	1.00	22.68	AAAA
ATOM	959	O	THR	A	134	-11.116	16.368	17.328	1.00	21.38	AAAA

ATOM	960	N	ASN	A	135	-9.927	15.267	15.771	1.00	23.98	AAAA
ATOM	961	CA	ASN	A	135	-8.636	15.623	16.358	1.00	24.64	AAAA
ATOM	962	CB	ASN	A	135	-7.488	14.936	15.597	1.00	24.49	AAAA
ATOM	963	CG	ASN	A	135	-7.020	13.638	16.264	1.00	25.25	AAAA
ATOM	964	OD1	ASN	A	135	-6.267	12.856	15.668	1.00	25.70	AAAA
ATOM	965	ND2	ASN	A	135	-7.445	13.415	17.504	1.00	22.51	AAAA
ATOM	966	C	ASN	A	135	-8.421	17.135	16.349	1.00	25.19	AAAA
ATOM	967	O	ASN	A	135	-7.890	17.702	17.301	1.00	24.79	AAAA
ATOM	968	N	LYS	A	136	-8.839	17.792	15.274	1.00	26.78	AAAA
ATOM	969	CA	LYS	A	136	-8.661	19.234	15.177	1.00	28.71	AAAA
ATOM	970	CB	LYS	A	136	-9.165	19.743	13.828	1.00	30.84	AAAA
ATOM	971	CG	LYS	A	136	-8.816	21.195	13.563	1.00	34.68	AAAA
ATOM	972	CD	LYS	A	136	-9.206	21.596	12.148	1.00	36.19	AAAA
ATOM	973	CE	LYS	A	136	-8.810	23.033	11.846	1.00	37.78	AAAA
ATOM	974	NZ	LYS	A	136	-9.124	23.414	10.432	1.00	40.33	AAAA
ATOM	975	C	LYS	A	136	-9.370	19.981	16.304	1.00	28.66	AAAA
ATOM	976	O	LYS	A	136	-8.803	20.900	16.902	1.00	28.47	AAAA
ATOM	977	N	TRP	A	137	-10.606	19.589	16.596	1.00	28.05	AAAA
ATOM	978	CA	TRP	A	137	-11.363	20.243	17.656	1.00	28.85	AAAA
ATOM	979	CB	TRP	A	137	-12.855	19.921	17.516	1.00	31.86	AAAA
ATOM	980	CG	TRP	A	137	-13.485	20.502	16.282	1.00	34.71	AAAA
ATOM	981	CD2	TRP	A	137	-14.788	20.206	15.755	1.00	36.70	AAAA
ATOM	982	CE2	TRP	A	137	-14.982	21.036	14.630	1.00	37.21	AAAA
ATOM	983	CE3	TRP	A	137	-15.811	19.321	16.130	1.00	38.46	AAAA
ATOM	984	CD1	TRP	A	137	-12.959	21.466	15.471	1.00	36.22	AAAA
ATOM	985	NE1	TRP	A	137	-13.851	21.794	14.480	1.00	36.96	AAAA
ATOM	986	CZ2	TRP	A	137	-16.160	21.010	13.869	1.00	38.57	AAAA
ATOM	987	CZ3	TRP	A	137	-16.986	19.295	15.373	1.00	39.12	AAAA
ATOM	988	CH2	TRP	A	137	-17.148	20.136	14.255	1.00	39.31	AAAA
ATOM	989	C	TRP	A	137	-10.868	19.803	19.029	1.00	28.01	AAAA
ATOM	990	O	TRP	A	137	-10.763	20.605	19.955	1.00	27.04	AAAA
ATOM	991	N	LEU	A	138	-10.548	18.520	19.143	1.00	27.31	AAAA
ATOM	992	CA	LEU	A	138	-10.072	17.943	20.393	1.00	26.35	AAAA
ATOM	993	CB	LEU	A	138	-9.879	16.444	20.174	1.00	27.79	AAAA
ATOM	994	CG	LEU	A	138	-10.054	15.384	21.262	1.00	30.24	AAAA
ATOM	995	CD1	LEU	A	138	-11.263	15.650	22.142	1.00	29.67	AAAA
ATOM	996	CD2	LEU	A	138	-10.178	14.036	20.562	1.00	30.06	AAAA
ATOM	997	C	LEU	A	138	-8.772	18.609	20.834	1.00	25.34	AAAA
ATOM	998	O	LEU	A	138	-8.532	18.814	22.030	1.00	23.81	AAAA
ATOM	999	N	ALA	A	139	-7.931	18.953	19.865	1.00	26.03	AAAA
ATOM	1000	CA	ALA	A	139	-6.657	19.595	20.160	1.00	26.05	AAAA
ATOM	1001	CB	ALA	A	139	-5.918	19.934	18.858	1.00	26.98	AAAA
ATOM	1002	C	ALA	A	139	-6.847	20.858	21.002	1.00	26.86	AAAA
ATOM	1003	O	ALA	A	139	-5.929	21.286	21.697	1.00	26.11	AAAA
ATOM	1004	N	LYS	A	140	-8.044	21.439	20.952	1.00	26.32	AAAA
ATOM	1005	CA	LYS	A	140	-8.329	22.649	21.716	1.00	26.90	AAAA
ATOM	1006	CB	LYS	A	140	-9.644	23.276	21.238	1.00	29.14	AAAA
ATOM	1007	CG	LYS	A	140	-9.665	23.595	19.749	1.00	31.62	AAAA
ATOM	1008	CD	LYS	A	140	-8.523	24.513	19.364	1.00	35.02	AAAA
ATOM	1009	CE	LYS	A	140	-8.811	25.975	19.704	1.00	37.44	AAAA
ATOM	1010	NZ	LYS	A	140	-9.865	26.555	18.812	1.00	40.43	AAAA
ATOM	1011	C	LYS	A	140	-8.395	22.414	23.230	1.00	25.59	AAAA
ATOM	1012	O	LYS	A	140	-8.333	23.361	24.004	1.00	24.94	AAAA
ATOM	1013	N	ILE	A	141	-8.526	21.159	23.649	1.00	24.13	AAAA
ATOM	1014	CA	ILE	A	141	-8.587	20.844	25.075	1.00	23.31	AAAA
ATOM	1015	CB	ILE	A	141	-9.971	20.270	25.477	1.00	22.85	AAAA
ATOM	1016	CG2	ILE	A	141	-11.046	21.355	25.372	1.00	23.88	AAAA
ATOM	1017	CG1	ILE	A	141	-10.313	19.071	24.595	1.00	23.34	AAAA
ATOM	1018	CD1	ILE	A	141	-11.574	18.339	25.012	1.00	25.61	AAAA
ATOM	1019	C	ILE	A	141	-7.524	19.822	25.482	1.00	23.06	AAAA
ATOM	1020	O	ILE	A	141	-7.427	19.450	26.655	1.00	22.52	AAAA
ATOM	1021	N	ALA	A	142	-6.724	19.375	24.520	1.00	21.80	AAAA
ATOM	1022	CA	ALA	A	142	-5.695	18.379	24.803	1.00	21.97	AAAA
ATOM	1023	CB	ALA	A	142	-5.231	17.739	23.495	1.00	20.41	AAAA
ATOM	1024	C	ALA	A	142	-4.491	18.924	25.580	1.00	21.11	AAAA
ATOM	1025	O	ALA	A	142	-4.132	20.094	25.465	1.00	22.76	AAAA

ATOM	1026	N	THR	A	143	-3.887	18.056	26.384	1.00	21.92	AAAA
ATOM	1027	CA	THR	A	143	-2.707	18.392	27.178	1.00	22.64	AAAA
ATOM	1028	CB	THR	A	143	-2.598	17.450	28.400	1.00	23.91	AAAA
ATOM	1029	OG1	THR	A	143	-3.751	17.635	29.232	1.00	25.42	AAAA
ATOM	1030	CG2	THR	A	143	-1.329	17.735	29.209	1.00	24.48	AAAA
ATOM	1031	C	THR	A	143	-1.454	18.235	26.312	1.00	22.79	AAAA
ATOM	1032	O	THR	A	143	-0.444	18.910	26.517	1.00	23.30	AAAA
ATOM	1033	N	LYS	A	144	-1.525	17.341	25.335	1.00	23.20	AAAA
ATOM	1034	CA	LYS	A	144	-0.398	17.106	24.440	1.00	25.09	AAAA
ATOM	1035	CB	LYS	A	144	0.565	16.083	25.049	1.00	25.01	AAAA
ATOM	1036	CG	LYS	A	144	1.706	15.658	24.129	1.00	28.28	AAAA
ATOM	1037	CD	LYS	A	144	2.604	16.838	23.747	1.00	27.48	AAAA
ATOM	1038	CE	LYS	A	144	3.818	16.373	22.946	1.00	29.11	AAAA
ATOM	1039	NZ	LYS	A	144	4.722	17.507	22.587	1.00	28.97	AAAA
ATOM	1040	C	LYS	A	144	-0.896	16.595	23.102	1.00	24.77	AAAA
ATOM	1041	O	LYS	A	144	-1.688	15.660	23.039	1.00	24.45	AAAA
ATOM	1042	N	VAL	A	145	-0.432	17.218	22.030	1.00	24.92	AAAA
ATOM	1043	CA	VAL	A	145	-0.830	16.793	20.701	1.00	25.14	AAAA
ATOM	1044	CB	VAL	A	145	-1.510	17.938	19.919	1.00	24.18	AAAA
ATOM	1045	CG1	VAL	A	145	-2.023	17.418	18.591	1.00	24.71	AAAA
ATOM	1046	CG2	VAL	A	145	-2.658	18.528	20.740	1.00	25.82	AAAA
ATOM	1047	C	VAL	A	145	0.420	16.356	19.950	1.00	25.49	AAAA
ATOM	1048	O	VAL	A	145	1.449	17.034	19.995	1.00	25.76	AAAA
ATOM	1049	N	MET	A	146	0.324	15.208	19.289	1.00	26.18	AAAA
ATOM	1050	CA	MET	A	146	1.421	14.654	18.503	1.00	26.41	AAAA
ATOM	1051	CB	MET	A	146	2.000	13.396	19.172	1.00	26.85	AAAA
ATOM	1052	CG	MET	A	146	2.826	13.653	20.430	1.00	25.85	AAAA
ATOM	1053	SD	MET	A	146	3.306	12.116	21.269	1.00	28.45	AAAA
ATOM	1054	CE	MET	A	146	1.827	11.741	22.217	1.00	26.47	AAAA
ATOM	1055	C	MET	A	146	0.860	14.293	17.131	1.00	27.20	AAAA
ATOM	1056	O	MET	A	146	-0.311	13.934	16.998	1.00	25.68	AAAA
ATOM	1057	N	GLN	A	147	1.701	14.395	16.111	1.00	28.03	AAAA
ATOM	1058	CA	GLN	A	147	1.294	14.091	14.748	1.00	28.39	AAAA
ATOM	1059	CB	GLN	A	147	1.067	15.388	13.979	1.00	28.65	AAAA
ATOM	1060	CG	GLN	A	147	2.203	16.371	14.142	1.00	30.13	AAAA
ATOM	1061	CD	GLN	A	147	2.006	17.653	13.360	1.00	29.84	AAAA
ATOM	1062	OE1	GLN	A	147	2.730	18.629	13.565	1.00	32.18	AAAA
ATOM	1063	NE2	GLN	A	147	1.036	17.657	12.453	1.00	29.40	AAAA
ATOM	1064	C	GLN	A	147	2.394	13.274	14.085	1.00	29.45	AAAA
ATOM	1065	O	GLN	A	147	3.570	13.420	14.424	1.00	29.21	AAAA
ATOM	1066	N	ALA	A	148	2.010	12.412	13.150	1.00	29.90	AAAA
ATOM	1067	CA	ALA	A	148	2.975	11.563	12.461	1.00	31.39	AAAA
ATOM	1068	CB	ALA	A	148	2.254	10.468	11.690	1.00	30.97	AAAA
ATOM	1069	C	ALA	A	148	3.846	12.373	11.514	1.00	32.66	AAAA
ATOM	1070	O	ALA	A	148	5.071	12.231	11.517	1.00	32.76	AAAA
ATOM	1071	N	PHE	A	149	3.205	13.220	10.712	1.00	33.44	AAAA
ATOM	1072	CA	PHE	A	149	3.903	14.059	9.744	1.00	35.09	AAAA
ATOM	1073	CB	PHE	A	149	3.367	13.814	8.332	1.00	34.59	AAAA
ATOM	1074	CG	PHE	A	149	3.200	12.367	7.985	1.00	35.35	AAAA
ATOM	1075	CD1	PHE	A	149	1.935	11.789	7.958	1.00	34.17	AAAA
ATOM	1076	CD2	PHE	A	149	4.304	11.579	7.685	1.00	34.88	AAAA
ATOM	1077	CE1	PHE	A	149	1.771	10.448	7.637	1.00	34.20	AAAA
ATOM	1078	CE2	PHE	A	149	4.148	10.236	7.364	1.00	36.09	AAAA
ATOM	1079	CZ	PHE	A	149	2.878	9.670	7.340	1.00	35.09	AAAA
ATOM	1080	C	PHE	A	149	3.719	15.536	10.056	1.00	36.17	AAAA
ATOM	1081	O	PHE	A	149	2.697	15.939	10.606	1.00	37.06	AAAA
ATOM	1082	N	PRO	A	150	4.709	16.370	9.704	1.00	37.23	AAAA
ATOM	1083	CD	PRO	A	150	6.002	16.078	9.056	1.00	37.75	AAAA
ATOM	1084	CA	PRO	A	150	4.569	17.803	9.975	1.00	38.03	AAAA
ATOM	1085	CB	PRO	A	150	5.967	18.341	9.682	1.00	38.69	AAAA
ATOM	1086	CG	PRO	A	150	6.432	17.448	8.569	1.00	38.52	AAAA
ATOM	1087	C	PRO	A	150	3.510	18.369	9.028	1.00	38.18	AAAA
ATOM	1088	O	PRO	A	150	3.355	17.878	7.912	1.00	38.42	AAAA
ATOM	1089	N	GLY	A	151	2.763	19.374	9.475	1.00	38.74	AAAA
ATOM	1090	CA	GLY	A	151	1.749	19.952	8.609	1.00	38.66	AAAA
ATOM	1091	C	GLY	A	151	0.300	19.705	8.996	1.00	38.69	AAAA

ATOM	1092	O	GLY	A	151	-0.571	20.502	8.645	1.00	38.08	AAAA
ATOM	1093	N	ALA	A	152	0.024	18.666	9.689	1.00	38.70	AAAA
ATOM	1094	CA	ALA	A	152	-1.343	18.311	10.112	1.00	38.90	AAAA
ATOM	1095	CB	ALA	A	152	-1.402	16.980	10.859	1.00	38.46	AAAA
ATOM	1096	C	ALA	A	152	-1.729	19.461	11.032	1.00	39.30	AAAA
ATOM	1097	O	ALA	A	152	-2.753	20.114	10.838	1.00	40.05	AAAA
ATOM	1098	N	PHE	A	153	-0.887	19.700	12.031	1.00	39.42	AAAA
ATOM	1099	CA	PHE	A	153	-1.084	20.795	12.971	1.00	39.90	AAAA
ATOM	1100	CB	PHE	A	153	-1.209	20.286	14.409	1.00	39.04	AAAA
ATOM	1101	CG	PHE	A	153	-2.478	19.535	14.685	1.00	38.06	AAAA
ATOM	1102	CD1	PHE	A	153	-2.571	18.175	14.419	1.00	36.71	AAAA
ATOM	1103	CD2	PHE	A	153	-3.582	20.190	15.228	1.00	37.52	AAAA
ATOM	1104	CE1	PHE	A	153	-3.747	17.475	14.692	1.00	36.39	AAAA
ATOM	1105	CE2	PHE	A	153	-4.761	19.500	15.502	1.00	36.08	AAAA
ATOM	1106	CZ	PHE	A	153	-4.842	18.140	15.235	1.00	36.20	AAAA
ATOM	1107	C	PHE	A	153	0.143	21.696	12.865	1.00	40.75	AAAA
ATOM	1108	O	PHE	A	153	1.238	21.228	12.543	1.00	41.03	AAAA
ATOM	1109	N	PRO	A	154	-0.026	23.001	13.128	1.00	41.05	AAAA
ATOM	1110	CD	PRO	A	154	-1.328	23.667	13.304	1.00	41.17	AAAA
ATOM	1111	CA	PRO	A	154	1.052	23.992	13.068	1.00	41.57	AAAA
ATOM	1112	CB	PRO	A	154	0.339	25.292	13.428	1.00	41.69	AAAA
ATOM	1113	CG	PRO	A	154	-1.024	25.081	12.876	1.00	41.76	AAAA
ATOM	1114	C	PRO	A	154	2.260	23.744	13.975	1.00	42.12	AAAA
ATOM	1115	O	PRO	A	154	3.400	23.833	13.515	1.00	43.15	AAAA
ATOM	1116	N	ASN	A	155	2.023	23.432	15.249	1.00	41.75	AAAA
ATOM	1117	CA	ASN	A	155	3.135	23.230	16.180	1.00	41.57	AAAA
ATOM	1118	CB	ASN	A	155	3.180	24.389	17.179	1.00	44.02	AAAA
ATOM	1119	CG	ASN	A	155	2.961	25.736	16.522	1.00	45.69	AAAA
ATOM	1120	OD1	ASN	A	155	1.862	26.045	16.058	1.00	47.64	AAAA
ATOM	1121	ND2	ASN	A	155	4.010	26.545	16.475	1.00	47.43	AAAA
ATOM	1122	C	ASN	A	155	3.193	21.921	16.970	1.00	40.83	AAAA
ATOM	1123	O	ASN	A	155	3.973	21.814	17.917	1.00	41.17	AAAA
ATOM	1124	N	ALA	A	156	2.390	20.929	16.601	1.00	38.83	AAAA
ATOM	1125	CA	ALA	A	156	2.400	19.658	17.326	1.00	37.19	AAAA
ATOM	1126	CB	ALA	A	156	1.203	18.811	16.909	1.00	36.03	AAAA
ATOM	1127	C	ALA	A	156	3.698	18.882	17.090	1.00	35.95	AAAA
ATOM	1128	O	ALA	A	156	4.206	18.834	15.971	1.00	35.55	AAAA
ATOM	1129	N	GLU	A	157	4.233	18.275	18.146	1.00	35.08	AAAA
ATOM	1130	CA	GLU	A	157	5.464	17.505	18.022	1.00	33.77	AAAA
ATOM	1131	CB	GLU	A	157	5.848	16.881	19.373	1.00	34.33	AAAA
ATOM	1132	CG	GLU	A	157	7.175	16.124	19.352	1.00	34.59	AAAA
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ATOM	1352	CG1	VAL	A	186	6.574	-2.124	-9.656	1.00	21.27
AAAA										
ATOM	1353	CG2	VAL	A	186	8.689	-2.252	-11.001	1.00	22.25
AAAA										
ATOM	1354	C	VAL	A	186	7.563	-4.294	-7.942	1.00	20.09
AAAA										
ATOM	1355	O	VAL	A	186	7.064	-5.330	-8.361	1.00	20.16
AAAA										
ATOM	1356	N	LEU	A	187	7.325	-3.807	-6.735	1.00	20.75
AAAA										
ATOM	1357	CA	LEU	A	187	6.421	-4.462	-5.801	1.00	21.10
AAAA										
ATOM	1358	CB	LEU	A	187	6.979	-4.363	-4.379	1.00	22.77
AAAA										
ATOM	1359	CG	LEU	A	187	6.492	-5.359	-3.316	1.00	24.90
AAAA										
ATOM	1360	CD1	LEU	A	187	6.763	-4.768	-1.932	1.00	23.74
AAAA										
ATOM	1361	CD2	LEU	A	187	5.027	-5.651	-3.487	1.00	27.67
AAAA										
ATOM	1362	C	LEU	A	187	5.104	-3.691	-5.871	1.00	21.37
AAAA										
ATOM	1363	O	LEU	A	187	5.078	-2.491	-5.585	1.00	21.09
AAAA										
ATOM	1364	N	VAL	A	188	4.034	-4.377	-6.262	1.00	21.43
AAAA										
ATOM	1365	CA	VAL	A	188	2.706	-3.774	-6.355	1.00	22.58
AAAA										
ATOM	1366	CB	VAL	A	188	1.988	-4.190	-7.657	1.00	22.95
AAAA										
ATOM	1367	CG1	VAL	A	188	0.643	-3.488	-7.765	1.00	22.98
AAAA										
ATOM	1368	CG2	VAL	A	188	2.853	-3.842	-8.855	1.00	23.03
AAAA										
ATOM	1369	C	VAL	A	188	1.891	-4.267	-5.161	1.00	22.98
AAAA										
ATOM	1370	O	VAL	A	188	1.603	-5.456	-5.051	1.00	22.38
AAAA										
ATOM	1371	N	VAL	A	189	1.534	-3.349	-4.267	1.00	23.91
AAAA										
ATOM	1372	CA	VAL	A	189	0.779	-3.706	-3.070	1.00	25.11
AAAA										
ATOM	1373	CB	VAL	A	189	1.523	-3.237	-1.800	1.00	25.30
AAAA										
ATOM	1374	CG1	VAL	A	189	0.740	-3.635	-0.549	1.00	23.23
AAAA										
ATOM	1375	CG2	VAL	A	189	2.915	-3.828	-1.773	1.00	22.20
AAAA										
ATOM	1376	C	VAL	A	189	-0.619	-3.096	-3.080	1.00	26.20
AAAA										
ATOM	1377	O	VAL	A	189	-0.770	-1.879	-3.186	1.00	26.94
AAAA										
ATOM	1378	N	GLY	A	190	-1.629	-3.955	-2.975	1.00	27.50
AAAA										

ATOM AAAA	1379	CA	GLY A 190	-3.007	-3.505	-2.966	1.00	30.27
ATOM AAAA	1380	C	GLY A 190	-3.720	-3.736	-1.641	1.00	32.15
ATOM AAAA	1381	O	GLY A 190	-4.896	-3.403	-1.499	1.00	32.00
ATOM AAAA	1382	N	GLY A 191	-3.016	-4.299	-0.664	1.00	32.97
ATOM AAAA	1383	CA	GLY A 191	-3.640	-4.550	0.624	1.00	34.29
ATOM AAAA	1384	C	GLY A 191	-4.507	-5.794	0.607	1.00	34.92
ATOM AAAA	1385	O	GLY A 191	-4.741	-6.388	-0.444	1.00	34.34
ATOM AAAA	1386	N	SER A 192	-4.996	-6.183	1.778	1.00	36.47
ATOM AAAA	1387	CA	SER A 192	-5.827	-7.377	1.910	1.00	38.39
ATOM AAAA	1388	CB	SER A 192	-6.389	-7.460	3.335	1.00	39.07
ATOM AAAA	1389	OG	SER A 192	-7.124	-6.291	3.658	1.00	41.25
ATOM AAAA	1390	C	SER A 192	-6.974	-7.472	0.903	1.00	38.69
ATOM AAAA	1391	O	SER A 192	-7.293	-8.557	0.410	1.00	38.58
ATOM AAAA	1392	N	GLN A 193	-7.599	-6.344	0.595	1.00	38.60
ATOM AAAA	1393	CA	GLN A 193	-8.715	-6.367	-0.339	1.00	39.91
ATOM AAAA	1394	CB	GLN A 193	-9.787	-5.367	0.110	1.00	41.97
ATOM AAAA	1395	CG	GLN A 193	-10.354	-5.679	1.497	1.00	43.94
ATOM AAAA	1396	CD	GLN A 193	-10.790	-7.135	1.640	1.00	45.71
ATOM AAAA	1397	OE1	GLN A 193	-11.677	-7.607	0.922	1.00	46.93
ATOM AAAA	1398	NE2	GLN A 193	-10.162	-7.853	2.567	1.00	45.80
ATOM AAAA	1399	C	GLN A 193	-8.298	-6.098	-1.781	1.00	39.31
ATOM AAAA	1400	O	GLN A 193	-9.076	-6.320	-2.708	1.00	39.52
ATOM AAAA	1401	N	GLY A 194	-7.064	-5.642	-1.961	1.00	38.40
ATOM AAAA	1402	CA	GLY A 194	-6.560	-5.358	-3.291	1.00	38.11
ATOM AAAA	1403	C	GLY A 194	-6.961	-3.987	-3.797	1.00	37.62
ATOM AAAA	1404	O	GLY A 194	-7.904	-3.382	-3.291	1.00	37.80
ATOM AAAA	1405	N	ALA A 195	-6.228	-3.489	-4.787	1.00	36.62
ATOM AAAA	1406	CA	ALA A 195	-6.513	-2.191	-5.387	1.00	36.35
ATOM AAAA	1407	CB	ALA A 195	-5.290	-1.291	-5.305	1.00	35.75
ATOM AAAA	1408	C	ALA A 195	-6.898	-2.437	-6.842	1.00	36.61
ATOM AAAA	1409	O	ALA A 195	-6.038	-2.519	-7.717	1.00	35.93
ATOM AAAA	1410	N	ARG A 196	-8.198	-2.566	-7.080	1.00	36.94
ATOM AAAA	1411	CA	ARG A 196	-8.741	-2.828	-8.412	1.00	38.03

ATOM	1412	CB	ARG	A	196	-10.229	-2.466	-8.450	1.00	40.33
AAAA										
ATOM	1413	CG	ARG	A	196	-10.526	-0.968	-8.375	1.00	44.08
AAAA										
ATOM	1414	CD	ARG	A	196	-9.935	-0.306	-7.129	1.00	46.46
AAAA										
ATOM	1415	NE	ARG	A	196	-10.381	-0.949	-5.894	1.00	48.33
AAAA										
ATOM	1416	CZ	ARG	A	196	-10.199	-0.439	-4.682	1.00	48.85
AAAA										
ATOM	1417	NH1	ARG	A	196	-9.581	0.725	-4.538	1.00	49.51
AAAA										
ATOM	1418	NH2	ARG	A	196	-10.636	-1.093	-3.615	1.00	49.95
AAAA										
ATOM	1419	C	ARG	A	196	-8.023	-2.120	-9.558	1.00	37.11
AAAA										
ATOM	1420	O	ARG	A	196	-7.729	-2.736	-10.583	1.00	36.96
AAAA										
ATOM	1421	N	ILE	A	197	-7.739	-0.834	-9.392	1.00	35.89
AAAA										
ATOM	1422	CA	ILE	A	197	-7.071	-0.091	-10.448	1.00	35.67
AAAA										
ATOM	1423	CB	ILE	A	197	-7.049	1.427	-10.161	1.00	36.70
AAAA										
ATOM	1424	CG2	ILE	A	197	-6.221	1.726	-8.918	1.00	36.91
AAAA										
ATOM	1425	CG1	ILE	A	197	-6.485	2.162	-11.381	1.00	36.95
AAAA										
ATOM	1426	CD1	ILE	A	197	-6.529	3.661	-11.272	1.00	38.71
AAAA										
ATOM	1427	C	ILE	A	197	-5.644	-0.580	-10.694	1.00	34.73
AAAA										
ATOM	1428	O	ILE	A	197	-5.178	-0.575	-11.833	1.00	33.53
AAAA										
ATOM	1429	N	LEU	A	198	-4.948	-0.992	-9.638	1.00	32.35
AAAA										
ATOM	1430	CA	LEU	A	198	-3.588	-1.494	-9.813	1.00	31.48
AAAA										
ATOM	1431	CB	LEU	A	198	-2.862	-1.633	-8.467	1.00	31.03
AAAA										
ATOM	1432	CG	LEU	A	198	-2.548	-0.342	-7.704	1.00	32.00
AAAA										
ATOM	1433	CD1	LEU	A	198	-1.773	-0.688	-6.442	1.00	30.82
AAAA										
ATOM	1434	CD2	LEU	A	198	-1.734	0.607	-8.566	1.00	30.86
AAAA										
ATOM	1435	C	LEU	A	198	-3.668	-2.850	-10.501	1.00	29.72
AAAA										
ATOM	1436	O	LEU	A	198	-2.837	-3.173	-11.344	1.00	29.46
AAAA										
ATOM	1437	N	ASN	A	199	-4.678	-3.639	-10.150	1.00	28.63
AAAA										
ATOM	1438	CA	ASN	A	199	-4.848	-4.952	-10.758	1.00	28.66
AAAA										
ATOM	1439	CB	ASN	A	199	-5.975	-5.724	-10.066	1.00	27.71
AAAA										
ATOM	1440	CG	ASN	A	199	-5.641	-6.069	-8.632	1.00	26.12
AAAA										
ATOM	1441	OD1	ASN	A	199	-4.501	-5.904	-8.200	1.00	24.15
AAAA										
ATOM	1442	ND2	ASN	A	199	-6.631	-6.553	-7.884	1.00	24.90
AAAA										
ATOM	1443	C	ASN	A	199	-5.144	-4.841	-12.248	1.00	29.87
AAAA										
ATOM	1444	O	ASN	A	199	-4.834	-5.747	-13.024	1.00	30.26
AAAA										

ATOM AAAA	1445	N	GLN	A	200	-5.746	-3.725	-12.644	1.00 31.15
ATOM AAAA	1446	CA	GLN	A	200	-6.085	-3.498	-14.044	1.00 33.06
ATOM AAAA	1447	CB	GLN	A	200	-7.396	-2.706	-14.145	1.00 34.24
ATOM AAAA	1448	CG	GLN	A	200	-8.590	-3.368	-13.471	1.00 38.64
ATOM AAAA	1449	CD	GLN	A	200	-8.923	-4.734	-14.050	1.00 41.05
ATOM AAAA	1450	OE1	GLN	A	200	-9.131	-4.879	-15.256	1.00 43.10
ATOM AAAA	1451	NE2	GLN	A	200	-8.983	-5.745	-13.185	1.00 43.12
ATOM AAAA	1452	C	GLN	A	200	-4.989	-2.753	-14.812	1.00 32.52
ATOM AAAA	1453	O	GLN	A	200	-4.809	-2.970	-16.008	1.00 34.23
ATOM AAAA	1454	N	THR	A	201	-4.247	-1.895	-14.120	1.00 31.87
ATOM AAAA	1455	CA	THR	A	201	-3.207	-1.092	-14.756	1.00 31.72
ATOM AAAA	1456	CB	THR	A	201	-3.046	0.245	-13.999	1.00 32.41
ATOM AAAA	1457	OG1	THR	A	201	-4.307	0.931	-13.976	1.00 32.19
ATOM AAAA	1458	CG2	THR	A	201	-2.003	1.131	-14.668	1.00 32.29
ATOM AAAA	1459	C	THR	A	201	-1.817	-1.728	-14.925	1.00 32.02
ATOM AAAA	1460	O	THR	A	201	-1.206	-1.626	-15.991	1.00 31.47
ATOM AAAA	1461	N	MET	A	202	-1.320	-2.394	-13.892	1.00 30.61
ATOM AAAA	1462	CA	MET	A	202	0.019	-2.975	-13.963	1.00 30.10
ATOM AAAA	1463	CB	MET	A	202	0.430	-3.507	-12.592	1.00 29.71
ATOM AAAA	1464	CG	MET	A	202	0.564	-2.406	-11.548	1.00 28.99
ATOM AAAA	1465	SD	MET	A	202	1.518	-0.961	-12.098	1.00 31.46
ATOM AAAA	1466	CE	MET	A	202	3.184	-1.633	-12.184	1.00 29.20
ATOM AAAA	1467	C	MET	A	202	0.286	-4.022	-15.042	1.00 29.48
ATOM AAAA	1468	O	MET	A	202	1.389	-4.088	-15.568	1.00 29.15
ATOM AAAA	1469	N	PRO	A	203	-0.703	-4.863	-15.379	1.00 30.34
ATOM AAAA	1470	CD	PRO	A	203	-1.957	-5.186	-14.677	1.00 30.05
ATOM AAAA	1471	CA	PRO	A	203	-0.415	-5.849	-16.426	1.00 31.11
ATOM AAAA	1472	CB	PRO	A	203	-1.703	-6.654	-16.500	1.00 31.89
ATOM AAAA	1473	CG	PRO	A	203	-2.188	-6.623	-15.072	1.00 31.09
ATOM AAAA	1474	C	PRO	A	203	-0.103	-5.139	-17.746	1.00 33.02
ATOM AAAA	1475	O	PRO	A	203	0.800	-5.530	-18.490	1.00 33.16
ATOM AAAA	1476	N	GLN	A	204	-0.855	-4.081	-18.020	1.00 33.88
ATOM AAAA	1477	CA	GLN	A	204	-0.666	-3.314	-19.242	1.00 34.99

ATOM 1478 CB GLN A 204 -1.836 -2.347 -19.431 1.00 37.12
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ATOM 1479 CG GLN A 204 -3.177 -3.067 -19.538 1.00 40.86
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ATOM 1480 CD GLN A 204 -4.354 -2.121 -19.700 1.00 43.77
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ATOM 1481 OE1 GLN A 204 -4.406 -1.330 -20.647 1.00 45.55
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ATOM 1482 NE2 GLN A 204 -5.310 -2.198 -18.776 1.00 44.11
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ATOM 1483 C GLN A 204 0.659 -2.573 -19.190 1.00 33.42
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ATOM 1484 O GLN A 204 1.331 -2.431 -20.206 1.00 34.40
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ATOM 1485 N VAL A 205 1.045 -2.114 -18.002 1.00 32.44
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ATOM 1486 CA VAL A 205 2.313 -1.417 -17.836 1.00 30.42
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ATOM 1487 CB VAL A 205 2.466 -0.834 -16.408 1.00 31.72
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ATOM 1488 CG1 VAL A 205 3.907 -0.406 -16.169 1.00 28.58
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ATOM 1489 CG2 VAL A 205 1.544 0.356 -16.231 1.00 29.91
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ATOM 1490 C VAL A 205 3.446 -2.407 -18.086 1.00 30.65
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ATOM 1491 O VAL A 205 4.473 -2.062 -18.686 1.00 29.65
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ATOM 1492 N ALA A 206 3.255 -3.638 -17.616 1.00 29.08
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ATOM 1493 CA ALA A 206 4.253 -4.688 -17.796 1.00 30.43
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ATOM 1494 CB ALA A 206 3.763 -6.002 -17.169 1.00 27.77
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ATOM 1495 C ALA A 206 4.519 -4.886 -19.288 1.00 30.65
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ATOM 1496 O ALA A 206 5.668 -5.040 -19.709 1.00 30.70
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ATOM 1497 N ALA A 207 3.450 -4.879 -20.080 1.00 31.56
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ATOM 1498 CA ALA A 207 3.565 -5.053 -21.527 1.00 32.70
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ATOM 1499 CB ALA A 207 2.188 -4.997 -22.167 1.00 32.49
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ATOM 1500 C ALA A 207 4.470 -3.990 -22.145 1.00 32.72
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ATOM 1501 O ALA A 207 5.295 -4.284 -23.007 1.00 33.64
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ATOM 1502 N LYS A 208 4.321 -2.754 -21.692 1.00 33.07
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ATOM 1503 CA LYS A 208 5.112 -1.651 -22.216 1.00 33.20
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ATOM 1504 CB LYS A 208 4.477 -0.313 -21.814 1.00 35.14
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ATOM 1505 CG LYS A 208 3.199 0.044 -22.578 1.00 38.07
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ATOM 1506 CD LYS A 208 2.166 -1.062 -22.482 1.00 40.27
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ATOM 1507 CE LYS A 208 0.892 -0.731 -23.233 1.00 41.02
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ATOM 1508 NZ LYS A 208 -0.076 -1.857 -23.126 1.00 42.41
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ATOM 1509 C LYS A 208 6.571 -1.668 -21.779 1.00 32.58
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ATOM 1510 O LYS A 208 7.456 -1.274 -22.544 1.00 31.82
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ATOM 1511 N LEU A 209 6.829 -2.121 -20.556 1.00 30.72
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ATOM 1512 CA LEU A 209 8.193 -2.143 -20.042 1.00 30.48
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ATOM 1513 CB LEU A 209 8.191 -1.848 -18.535 1.00 29.34
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ATOM 1514 CG LEU A 209 7.596 -0.498 -18.107 1.00 31.02
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ATOM 1515 CD1 LEU A 209 7.779 -0.318 -16.605 1.00 29.42
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ATOM 1516 CD2 LEU A 209 8.273 0.641 -18.859 1.00 31.39
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ATOM 1517 C LEU A 209 8.970 -3.432 -20.315 1.00 29.73
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ATOM 1518 O LEU A 209 10.191 -3.455 -20.174 1.00 31.33
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ATOM 1519 N GLY A 210 8.269 -4.494 -20.698 1.00 29.76
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ATOM 1520 CA GLY A 210 8.924 -5.762 -20.986 1.00 29.99
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ATOM 1521 C GLY A 210 10.007 -6.188 -20.003 1.00 30.99
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ATOM 1522 O GLY A 210 9.788 -6.183 -18.789 1.00 30.80
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ATOM 1523 N ASP A 211 11.181 -6.536 -20.535 1.00 30.05
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ATOM 1524 CA ASP A 211 12.332 -6.999 -19.749 1.00 29.42
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ATOM 1525 CB ASP A 211 13.466 -7.479 -20.676 1.00 30.83
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ATOM 1526 CG ASP A 211 13.119 -8.735 -21.449 1.00 32.09
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ATOM 1527 OD1 ASP A 211 13.977 -9.193 -22.235 1.00 34.13
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ATOM 1528 OD2 ASP A 211 12.005 -9.269 -21.283 1.00 32.72
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ATOM 1529 C ASP A 211 12.960 -6.011 -18.776 1.00 29.03
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ATOM 1530 O ASP A 211 13.781 -6.417 -17.945 1.00 27.69
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ATOM 1531 N SER A 212 12.613 -4.730 -18.876 1.00 28.54
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ATOM 1532 CA SER A 212 13.204 -3.719 -18.002 1.00 27.61
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ATOM 1533 CB SER A 212 12.927 -2.308 -18.538 1.00 28.62
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ATOM 1534 OG SER A 212 11.546 -1.990 -18.498 1.00 30.84
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ATOM 1535 C SER A 212 12.759 -3.805 -16.542 1.00 26.31
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ATOM 1536 O SER A 212 13.395 -3.219 -15.666 1.00 25.39
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ATOM 1537 N VAL A 213 11.675 -4.528 -16.284 1.00 25.65
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ATOM 1538 CA VAL A 213 11.187 -4.671 -14.914 1.00 24.52
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ATOM 1539 CB VAL A 213 9.967 -3.747 -14.621 1.00 25.58
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ATOM 1540 CG1 VAL A 213 10.296 -2.298 -14.953 1.00 26.31
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ATOM 1541 CG2 VAL A 213 8.758 -4.225 -15.394 1.00 25.15
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ATOM 1542 C VAL A 213 10.751 -6.095 -14.607 1.00 23.77
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ATOM 1543 O VAL A 213 10.427 -6.874 -15.506 1.00 23.79
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ATOM 1544 N THR A 214 10.770 -6.432 -13.323 1.00 23.49
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ATOM 1545 CA THR A 214 10.326 -7.735 -12.861 1.00 21.50
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ATOM 1546 CB THR A 214 11.499 -8.600 -12.325 1.00 21.99
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ATOM 1547 OG1 THR A 214 10.987 -9.870 -11.909 1.00 23.56
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ATOM 1548 CG2 THR A 214 12.220 -7.921 -11.174 1.00 20.60
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ATOM 1549 C THR A 214 9.342 -7.362 -11.760 1.00 21.46
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ATOM 1550 O THR A 214 9.657 -6.567 -10.880 1.00 21.12
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ATOM 1551 N ILE A 215 8.150 -7.938 -11.827 1.00 21.73
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ATOM 1552 CA ILE A 215 7.083 -7.601 -10.894 1.00 22.01
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ATOM 1553 CB ILE A 215 5.831 -7.139 -11.688 1.00 22.41
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ATOM 1554 CG2 ILE A 215 4.707 -6.738 -10.734 1.00 22.94
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ATOM 1555 CG1 ILE A 215 6.198 -5.964 -12.599 1.00 22.71
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ATOM 1556 CD1 ILE A 215 5.078 -5.560 -13.545 1.00 21.71
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ATOM 1557 C ILE A 215 6.617 -8.685 -9.929 1.00 21.67
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ATOM 1558 O ILE A 215 6.600 -9.868 -10.257 1.00 20.14
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ATOM 1559 N TRP A 216 6.248 -8.247 -8.728 1.00 21.03
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ATOM 1560 CA TRP A 216 5.677 -9.121 -7.708 1.00 21.08
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ATOM 1561 CB TRP A 216 6.541 -9.186 -6.455 1.00 21.14
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ATOM 1562 CG TRP A 216 5.941 -10.063 -5.370 1.00 21.49
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ATOM 1563 CD2 TRP A 216 6.624 -10.588 -4.226 1.00 21.97
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ATOM 1564 CE2 TRP A 216 5.674 -11.309 -3.461 1.00 22.67
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ATOM 1565 CE3 TRP A 216 7.947 -10.521 -3.773 1.00 22.25
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ATOM 1566 CD1 TRP A 216 4.639 -10.478 -5.262 1.00 21.72
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ATOM 1567 NE1 TRP A 216 4.472 -11.231 -4.112 1.00 22.34
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ATOM 1568 CZ2 TRP A 216 6.011 -11.955 -2.265 1.00 24.81
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ATOM 1569 CZ3 TRP A 216 8.283 -11.166 -2.582 1.00 23.37
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ATOM 1570 CH2 TRP A 216 7.316 -11.872 -1.843 1.00 23.19
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ATOM 1571 C TRP A 216 4.401 -8.352 -7.396 1.00 21.75
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ATOM 1572 O TRP A 216 4.442 -7.330 -6.719 1.00 22.71
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ATOM 1574 CA HIS A 217 1.987 -8.185 -7.751 1.00 24.05
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ATOM 1575 CB HIS A 217 1.301 -8.167 -9.127 1.00 25.31
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ATOM 1576 CG HIS A 217 0.075 -7.312 -9.201 1.00 27.29
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ATOM 1578 ND1 HIS A 217 -0.146 -6.424 -10.233 1.00 28.22
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ATOM 1579 CE1 HIS A 217 -1.311 -5.828 -10.057 1.00 28.76
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ATOM 1580 NE2 HIS A 217 -1.856 -6.296 -8.947 1.00 27.39
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ATOM 1582 O HIS A 217 0.785 -10.059 -6.851 1.00 24.60
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ATOM 1585 CB GLN A 218 0.271 -8.181 -3.250 1.00 25.16
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ATOM 1590 C GLN A 218 -1.573 -8.134 -4.983 1.00 24.83
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ATOM 1591 O GLN A 218 -1.859 -6.960 -4.767 1.00 24.21
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ATOM 1594 CB SER A 219 -4.189 -9.704 -7.035 1.00 28.46
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ATOM 1595 OG SER A 219 -4.394 -10.949 -6.387 1.00 29.92
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ATOM 1596 C SER A 219 -4.887 -8.470 -5.034 1.00 29.52
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ATOM 1597 O SER A 219 -5.842 -7.745 -5.321 1.00 29.47
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ATOM 1607 CE LYS A 221 -11.955 -13.465 1.368 1.00 41.74
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ATOM 1616 CA SER A 223 -8.083 -11.691 -7.349 1.00 35.04
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ATOM 1617 CB SER A 223 -7.959 -10.175 -7.173 1.00 35.18
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ATOM 1635 OE1 GLN A 225 -8.418 -19.609 -10.952 1.00 44.03
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ATOM 1641 CB SER A 226 -8.865 -11.920 -12.251 1.00 34.12
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ATOM 1642 OG SER A 226 -8.460 -10.954 -11.300 1.00 36.16
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ATOM 1643 C SER A 226 -6.502 -11.926 -13.090 1.00 32.76
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ATOM 1644 O SER A 226 -6.343 -11.580 -14.260 1.00 32.64
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ATOM 1646 CA VAL A 227 -4.498 -10.737 -12.400 1.00 30.69
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ATOM 1647 CB VAL A 227 -3.942 -10.117 -11.102 1.00 29.27
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ATOM 1648 CG1 VAL A 227 -2.619 -9.413 -11.370 1.00 29.04
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ATOM 1649 CG2 VAL A 227 -4.951 -9.117 -10.546 1.00 29.09
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ATOM 1651 O VAL A 227 -2.716 -11.103 -13.973 1.00 29.50
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ATOM 1654 CB GLU A 228 -2.456 -15.108 -12.464 1.00 31.67
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ATOM 1658 OE2 GLU A 228 0.190 -15.280 -11.761 1.00 35.02
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ATOM 1659 C GLU A 228 -2.658 -13.944 -14.685 1.00 32.05
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ATOM 1660 O GLU A 228 -1.770 -13.942 -15.539 1.00 32.57
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ATOM 1663 CB GLN A 229 -5.896 -14.616 -16.359 1.00 35.59
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ATOM 1665 CD GLN A 229 -7.825 -15.665 -17.623 1.00 41.31
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ATOM 1667 NE2 GLN A 229 -8.516 -15.332 -16.538 1.00 43.19
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ATOM 1671 CA ALA A 230 -4.092 -10.542 -17.131 1.00 30.04
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ATOM 1672 CB ALA A 230 -4.453 -9.423 -16.165 1.00 30.37
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ATOM 1673 C ALA A 230 -2.649 -10.379 -17.598 1.00 29.65
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ATOM 1674 O ALA A 230 -2.392 -9.869 -18.689 1.00 29.50
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ATOM 1676 CA TYR A 231 -0.295 -10.707 -17.111 1.00 27.27
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ATOM 1678 CG TYR A 231 0.829 -9.898 -14.975 1.00 24.33
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ATOM 1679 CD1 TYR A 231 1.687 -8.866 -15.354 1.00 22.96
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ATOM 1680 CE1 TYR A 231 1.926 -7.786 -14.520 1.00 22.17
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ATOM 1681 CD2 TYR A 231 0.210 -9.817 -13.725 1.00 24.32
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ATOM 1682 CE2 TYR A 231 0.442 -8.737 -12.879 1.00 21.70
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ATOM 1683 CZ TYR A 231 1.298 -7.729 -13.281 1.00 21.49
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ATOM 1684 OH TYR A 231 1.532 -6.662 -12.466 1.00 18.68
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ATOM 1685 C TYR A 231 0.047 -11.618 -18.285 1.00 28.10
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ATOM 1686 O TYR A 231 0.834 -11.249 -19.163 1.00 27.39
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ATOM 1687 N ALA A 232 -0.547 -12.808 -18.297 1.00 28.86
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ATOM 1688 CA ALA A 232 -0.310 -13.775 -19.364 1.00 29.80
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ATOM 1689 CB ALA A 232 -1.013 -15.091 -19.046 1.00 30.32
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ATOM 1690 C ALA A 232 -0.814 -13.218 -20.694 1.00 30.76
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ATOM 1691 O ALA A 232 -0.147 -13.336 -21.725 1.00 30.92
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ATOM 1692 N GLU A 233 -1.996 -12.614 -20.662 1.00 31.01
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ATOM 1693 CA GLU A 233 -2.592 -12.034 -21.857 1.00 32.12
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ATOM 1694 CB GLU A 233 -4.051 -11.658 -21.579 1.00 33.81
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ATOM 1695 CG GLU A 233 -4.975 -12.871 -21.514 1.00 35.08
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ATOM 1696 CD GLU A 233 -6.402 -12.523 -21.117 1.00 37.70
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ATOM 1697 OE1 GLU A 233 -6.875 -11.419 -21.473 1.00 37.78
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ATOM 1698 OE2 GLU A 233 -7.056 -13.364 -20.461 1.00 37.69
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ATOM 1700 O GLU A 233 -1.825 -10.463 -23.508 1.00 32.48
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ATOM 1702 CA ALA A 234 -0.283 -9.022 -21.736 1.00 29.79
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ATOM 1703 CB ALA A 234 -0.089 -8.141 -20.505 1.00 30.39
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ATOM 1704 C ALA A 234 1.070 -9.501 -22.265 1.00 28.79
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ATOM 1705 O ALA A 234 1.934 -8.697 -22.604 1.00 28.46
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ATOM 1707 CA GLY A 235 2.484 -11.388 -22.807 1.00 26.98
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ATOM 1708 C GLY A 235 3.650 -11.387 -21.832 1.00 25.89
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ATOM 1709 O GLY A 235 4.798 -11.527 -22.253 1.00 25.26
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ATOM 1711 CA GLN A 236 4.419 -11.223 -19.518 1.00 24.12
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ATOM 1712 CB GLN A 236 4.652 -9.806 -18.977 1.00 24.66
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ATOM 1713 CG GLN A 236 5.116 -8.760 -20.003 1.00 25.88
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ATOM 1714 CD GLN A 236 6.454 -9.088 -20.647 1.00 26.71
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ATOM 1718 O GLN A 236 3.823 -11.696 -17.233 1.00 22.19
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ATOM 1719 N PRO A 237 3.740 -13.419 -18.679 1.00 22.50
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ATOM 1722 CB PRO A 237 2.998 -15.626 -18.531 1.00 22.52
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ATOM 1723 CG PRO A 237 4.105 -15.558 -19.543 1.00 23.54
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ATOM 1724 C PRO A 237 4.252 -14.695 -16.550 1.00 22.53
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ATOM 1725 O PRO A 237 3.845 -15.217 -15.512 1.00 23.09
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ATOM 1727 CA GLN A 238 6.539 -14.633 -15.726 1.00 22.49
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ATOM 1728 CB GLN A 238 7.947 -14.437 -16.304 1.00 22.24
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ATOM 1729 CG GLN A 238 8.376 -12.991 -16.520 1.00 21.45
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ATOM 1730 CD GLN A 238 7.727 -12.356 -17.736 1.00 22.77
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ATOM 1732 NE2 GLN A 238 7.881 -11.046 -17.870 1.00 22.96
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ATOM 1733 C GLN A 238 6.453 -13.856 -14.426 1.00 21.84
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ATOM 1734 O GLN A 238 7.059 -14.253 -13.427 1.00 21.75
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ATOM 1735 N HIS A 239 5.724 -12.748 -14.420 1.00 22.21
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ATOM 1736 CA HIS A 239 5.632 -11.963 -13.202 1.00 22.02
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ATOM 1737 CB HIS A 239 4.919 -10.638 -13.479 1.00 22.03
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ATOM 1738 CG HIS A 239 5.688 -9.734 -14.392 1.00 22.30
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ATOM 1739 CD2 HIS A 239 5.315 -9.057 -15.505 1.00 22.95
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ATOM 1740 ND1 HIS A 239 7.021 -9.445 -14.197 1.00 21.95
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ATOM 1741 CE1 HIS A 239 7.437 -8.628 -15.149 1.00 23.56
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ATOM 1742 NE2 HIS A 239 6.421 -8.378 -15.956 1.00 21.89
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ATOM 1743 C HIS A 239 4.937 -12.739 -12.092 1.00 20.83
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ATOM 1744 O HIS A 239 4.036 -13.538 -12.352 1.00 21.43
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ATOM 1745 N LYS A 240 5.381 -12.506 -10.858 1.00 21.17
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ATOM 1746 CA LYS A 240 4.819 -13.183 -9.687 1.00 22.02
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ATOM 1747 CB LYS A 240 5.840 -13.175 -8.543 1.00 21.72
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ATOM 1748 CG LYS A 240 5.420 -13.918 -7.257 1.00 22.71
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ATOM 1749 CD LYS A 240 6.462 -13.691 -6.163 1.00 23.02
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ATOM 1750 CE LYS A 240 6.155 -14.439 -4.855 1.00 22.89
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ATOM 1751 NZ LYS A 240 6.359 -15.920 -4.960 1.00 23.41
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ATOM 1752 C LYS A 240 3.545 -12.500 -9.214 1.00 21.50
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ATOM 1753 O LYS A 240 3.527 -11.288 -9.022 1.00 22.79
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ATOM 1754 N VAL A 241 2.490 -13.282 -9.012 1.00 23.27
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ATOM 1755 CA VAL A 241 1.219 -12.751 -8.527 1.00 23.82
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ATOM 1756 CB VAL A 241 0.111 -12.821 -9.598 1.00 23.97
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ATOM 1757 CG1 VAL A 241 -1.170 -12.185 -9.057 1.00 24.26
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ATOM 1758 CG2 VAL A 241 0.563 -12.105 -10.862 1.00 22.10
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ATOM 1759 C VAL A 241 0.751 -13.565 -7.323 1.00 23.52
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ATOM 1760 O VAL A 241 0.593 -14.781 -7.415 1.00 25.10
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ATOM 1762 CA THR A 242 0.083 -13.578 -4.991 1.00 25.34
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ATOM 1763 CB THR A 242 1.176 -13.635 -3.892 1.00 23.46
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ATOM 1764 OG1 THR A 242 1.633 -12.312 -3.590 1.00 24.62
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ATOM 1765 CG2 THR A 242 2.354 -14.482 -4.351 1.00 25.33
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ATOM 1766 C THR A 242 -1.144 -12.870 -4.435 1.00 26.25
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ATOM 1767 O THR A 242 -1.278 -11.645 -4.534 1.00 25.29
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ATOM 1768 N GLU A 243 -2.051 -13.647 -3.860 1.00 26.45
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ATOM 1769 CA GLU A 243 -3.256 -13.070 -3.293 1.00 28.18
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ATOM 1770 CB GLU A 243 -4.152 -14.184 -2.746 1.00 28.90
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ATOM 1771 CG GLU A 243 -5.463 -13.705 -2.156 1.00 32.51
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ATOM 1772 CD GLU A 243 -6.448 -14.845 -1.957 1.00 33.27
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ATOM 1773 OE1 GLU A 243 -6.002 -15.969 -1.646 1.00 33.05
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ATOM 1774 OE2 GLU A 243 -7.665 -14.612 -2.107 1.00 34.89
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ATOM	1778	CA	PHE	A	244	-1.509	-11.696	-0.208	1.00 29.32
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ATOM	1779	CB	PHE	A	244	-2.079	-12.202	1.122	1.00 31.34
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ATOM	1780	CG	PHE	A	244	-3.571	-12.360	1.139	1.00 32.25
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ATOM	1781	CD1	PHE	A	244	-4.406	-11.249	1.103	1.00 34.11
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ATOM	1782	CD2	PHE	A	244	-4.141	-13.623	1.246	1.00 33.07
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ATOM	1783	CE1	PHE	A	244	-5.794	-11.393	1.179	1.00 34.27
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ATOM	1784	CE2	PHE	A	244	-5.525	-13.780	1.323	1.00 34.74
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ATOM	1785	CZ	PHE	A	244	-6.353	-12.660	1.291	1.00 34.28
AAAA									
ATOM	1786	C	PHE	A	244	0.010	-11.759	-0.103	1.00 29.21
AAAA									
ATOM	1787	O	PHE	A	244	0.660	-12.503	-0.836	1.00 28.44
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ATOM	1788	N	ILE	A	245	0.560	-10.962	0.813	1.00 29.58
AAAA									
ATOM	1789	CA	ILE	A	245	1.993	-10.956	1.116	1.00 30.22
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ATOM	1790	CB	ILE	A	245	2.764	-9.766	0.503	1.00 29.45
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ATOM	1791	CG2	ILE	A	245	4.190	-9.741	1.060	1.00 27.25
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ATOM	1792	CG1	ILE	A	245	2.824	-9.887	-1.020	1.00 26.11
AAAA									
ATOM	1793	CD1	ILE	A	245	3.609	-8.774	-1.661	1.00 27.15
AAAA									
ATOM	1794	C	ILE	A	245	2.086	-10.822	2.631	1.00 32.52
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ATOM	1795	O	ILE	A	245	1.987	-9.720	3.176	1.00 32.53
AAAA									
ATOM	1796	N	ASP	A	246	2.271	-11.944	3.311	1.00 34.55
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ATOM	1797	CA	ASP	A	246	2.357	-11.926	4.763	1.00 36.92
AAAA									
ATOM	1798	CB	ASP	A	246	2.222	-13.350	5.304	1.00 40.29
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ATOM	1799	CG	ASP	A	246	0.831	-13.926	5.075	1.00 43.98
AAAA									
ATOM	1800	OD1	ASP	A	246	0.659	-15.159	5.218	1.00 46.68
AAAA									
ATOM	1801	OD2	ASP	A	246	-0.093	-13.143	4.760	1.00 45.65
AAAA									
ATOM	1802	C	ASP	A	246	3.650	-11.286	5.247	1.00 36.42
AAAA									
ATOM	1803	O	ASP	A	246	3.631	-10.384	6.092	1.00 37.48
AAAA									
ATOM	1804	N	ASP	A	247	4.771	-11.733	4.694	1.00 35.16
AAAA									
ATOM	1805	CA	ASP	A	247	6.069	-11.200	5.085	1.00 34.25
AAAA									
ATOM	1806	CB	ASP	A	247	7.145	-12.268	4.887	1.00 33.07
AAAA									
ATOM	1807	CG	ASP	A	247	8.461	-11.901	5.543	1.00 33.19
AAAA									

ATOM	1808	OD1	ASP	A	247	8.689	-10.700	5.802	1.00	31.85
AAAA										
ATOM	1809	OD2	ASP	A	247	9.277	-12.816	5.791	1.00	32.31
AAAA										
ATOM	1810	C	ASP	A	247	6.422	-9.949	4.275	1.00	34.18
AAAA										
ATOM	1811	O	ASP	A	247	7.241	-10.003	3.354	1.00	33.62
AAAA										
ATOM	1812	N	MET	A	248	5.801	-8.825	4.617	1.00	33.66
AAAA										
ATOM	1813	CA	MET	A	248	6.069	-7.577	3.916	1.00	33.29
AAAA										
ATOM	1814	CB	MET	A	248	5.192	-6.448	4.461	1.00	34.30
AAAA										
ATOM	1815	CG	MET	A	248	3.852	-6.314	3.757	1.00	36.70
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ATOM	1816	SD	MET	A	248	4.042	-5.940	1.987	1.00	40.22
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ATOM	1817	CE	MET	A	248	2.590	-6.667	1.361	1.00	39.66
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ATOM	1818	C	MET	A	248	7.533	-7.180	4.017	1.00	32.64
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ATOM	1820	N	ALA	A	249	8.166	-7.500	5.142	1.00	30.31
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AAAA										
ATOM	1824	O	ALA	A	249	11.277	-7.208	3.622	1.00	27.98
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ATOM	1828	C	ALA	A	250	10.624	-9.250	1.553	1.00	26.35
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ATOM	1837	CB	TYR	A	252	10.191	-4.033	2.131	1.00	26.30
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ATOM	1840	CE1	TYR	A	252	7.048	-2.395	3.547	1.00	30.51
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ATOM 1842 CE2 TYR A 252 6.821 -2.485 1.153 1.00 29.76
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ATOM 1843 CZ TYR A 252 6.322 -2.125 2.401 1.00 30.32
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ATOM 1844 OH TYR A 252 5.103 -1.492 2.515 1.00 29.75
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ATOM 1845 C TYR A 252 11.998 -4.972 0.694 1.00 25.22
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ATOM 1846 O TYR A 252 12.668 -4.106 0.139 1.00 24.57
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ATOM 1850 C ALA A 253 14.319 -6.560 -0.347 1.00 24.16
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ATOM 1851 O ALA A 253 15.325 -6.045 -0.831 1.00 26.29
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ATOM 1855 CG TRP A 254 12.534 -8.968 -4.304 1.00 21.21
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ATOM 1856 CD2 TRP A 254 11.508 -8.437 -5.155 1.00 20.22
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ATOM 1857 CE2 TRP A 254 11.766 -8.905 -6.463 1.00 20.36
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ATOM 1858 CE3 TRP A 254 10.397 -7.610 -4.939 1.00 20.38
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ATOM 1860 NE1 TRP A 254 12.895 -9.678 -6.404 1.00 22.48
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ATOM 1861 CZ2 TRP A 254 10.948 -8.573 -7.559 1.00 21.36
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ATOM 1862 CZ3 TRP A 254 9.582 -7.276 -6.030 1.00 21.09
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ATOM 1863 CH2 TRP A 254 9.867 -7.761 -7.323 1.00 20.78
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ATOM 1864 C TRP A 254 13.433 -6.468 -3.414 1.00 22.65
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ATOM 1865 O TRP A 254 14.218 -6.280 -4.345 1.00 23.19
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ATOM 1866 N ALA A 255 12.376 -5.692 -3.194 1.00 21.49
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ATOM 1870 O ALA A 255 13.844 -3.110 -3.469 1.00 21.35
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ATOM	1875	OD1	ASP	A	256	15.354	-3.417	-8.306	1.00 24.63
ATOM	1876	OD2	ASP	A	256	16.289	-2.328	-6.648	1.00 25.60
ATOM	1877	C	ASP	A	256	12.651	-0.397	-5.670	1.00 22.26
ATOM	1878	O	ASP	A	256	13.053	0.703	-5.300	1.00 22.77
ATOM	1879	N	VAL	A	257	11.379	-0.637	-5.968	1.00 23.20
ATOM	1880	CA	VAL	A	257	10.366	0.411	-5.914	1.00 23.31
ATOM	1881	CB	VAL	A	257	10.313	1.167	-7.267	1.00 23.63
ATOM	1882	CG1	VAL	A	257	9.950	0.206	-8.373	1.00 21.70
ATOM	1883	CG2	VAL	A	257	9.312	2.315	-7.205	1.00 23.86
ATOM	1884	C	VAL	A	257	8.997	-0.197	-5.607	1.00 23.39
ATOM	1885	O	VAL	A	257	8.735	-1.351	-5.933	1.00 22.20
ATOM	1886	N	VAL	A	258	8.127	0.587	-4.978	1.00 24.57
ATOM	1887	CA	VAL	A	258	6.792	0.114	-4.627	1.00 24.32
ATOM	1888	CB	VAL	A	258	6.590	0.100	-3.085	1.00 25.07
ATOM	1889	CG1	VAL	A	258	5.275	-0.596	-2.731	1.00 25.09
ATOM	1890	CG2	VAL	A	258	7.755	-0.599	-2.406	1.00 25.19
ATOM	1891	C	VAL	A	258	5.695	0.993	-5.228	1.00 24.77
ATOM	1892	O	VAL	A	258	5.806	2.220	-5.241	1.00 25.72
ATOM	1893	N	VAL	A	259	4.650	0.352	-5.738	1.00 24.90
ATOM	1894	CA	VAL	A	259	3.495	1.056	-6.291	1.00 24.40
ATOM	1895	CB	VAL	A	259	3.152	0.593	-7.713	1.00 24.26
ATOM	1896	CG1	VAL	A	259	1.928	1.371	-8.226	1.00 22.17
ATOM	1897	CG2	VAL	A	259	4.344	0.801	-8.628	1.00 21.85
ATOM	1898	C	VAL	A	259	2.351	0.653	-5.368	1.00 25.42
ATOM	1899	O	VAL	A	259	2.018	-0.528	-5.274	1.00 25.59
ATOM	1900	N	CYS	A	260	1.752	1.623	-4.685	1.00 25.57
ATOM	1901	CA	CYS	A	260	0.680	1.308	-3.750	1.00 26.61
ATOM	1902	CB	CYS	A	260	1.286	0.675	-2.495	1.00 25.90
ATOM	1903	SG	CYS	A	260	2.509	1.742	-1.683	1.00 29.42
ATOM	1904	C	CYS	A	260	-0.113	2.538	-3.330	1.00 27.15
ATOM	1905	O	CYS	A	260	0.221	3.664	-3.702	1.00 27.13
ATOM	1906	N	ARG	A	261	-1.164	2.306	-2.547	1.00 28.36

ATOM	1907	CA	ARG	A	261	-1.986	3.391	-2.023	1.00 29.99
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ATOM	1925	C	GLY	A	263	-1.510	5.663	4.680	1.00 29.40
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ATOM   1943  OG1 THR A 266      -0.066   1.315   3.697  1.00 27.63
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ATOM   1944  CG2 THR A 266       1.683   2.059   2.202  1.00 27.00
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ATOM   1970  CA  ILE A 270       7.711   2.763   3.158  1.00 28.64
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ATOM   1971  CB  ILE A 270       6.968   3.520   2.028  1.00 28.20
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ATOM   1972  CG2 ILE A 270       7.948   3.931   0.940  1.00 28.68
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ATOM	2029	CD2	PHE	A	279	2.751	5.817	-1.710	1.00 26.40
AAAA									
ATOM	2030	CE1	PHE	A	279	4.765	7.506	-0.821	1.00 27.90
AAAA									
ATOM	2031	CE2	PHE	A	279	3.549	5.439	-0.630	1.00 25.57
AAAA									
ATOM	2032	CZ	PHE	A	279	4.555	6.286	-0.186	1.00 25.90
AAAA									
ATOM	2033	C	PHE	A	279	0.765	6.773	-5.508	1.00 30.70
AAAA									
ATOM	2034	O	PHE	A	279	0.790	7.719	-6.294	1.00 30.85
AAAA									
ATOM	2035	N	VAL	A	280	-0.281	5.968	-5.367	1.00 31.23
AAAA									
ATOM	2036	CA	VAL	A	280	-1.523	6.161	-6.101	1.00 32.57
AAAA									
ATOM	2037	CB	VAL	A	280	-1.867	4.924	-6.954	1.00 33.12
AAAA									
ATOM	2038	CG1	VAL	A	280	-3.196	5.122	-7.661	1.00 32.63
AAAA									

ATOM	2039	CG2	VAL	A	280	-0.768	4.688	-7.979	1.00	33.54
AAAA										
ATOM	2040	C	VAL	A	280	-2.598	6.394	-5.036	1.00	33.46
AAAA										
ATOM	2041	O	VAL	A	280	-3.320	5.478	-4.643	1.00	32.49
AAAA										
ATOM	2042	N	PRO	A	281	-2.695	7.640	-4.546	1.00	34.67
AAAA										
ATOM	2043	CD	PRO	A	281	-1.917	8.789	-5.036	1.00	34.47
AAAA										
ATOM	2044	CA	PRO	A	281	-3.652	8.061	-3.518	1.00	36.79
AAAA										
ATOM	2045	CB	PRO	A	281	-3.475	9.578	-3.478	1.00	36.20
AAAA										
ATOM	2046	CG	PRO	A	281	-2.060	9.772	-3.909	1.00	36.53
AAAA										
ATOM	2047	C	PRO	A	281	-5.097	7.676	-3.801	1.00	38.44
AAAA										
ATOM	2048	O	PRO	A	281	-5.564	7.763	-4.936	1.00	38.62
AAAA										
ATOM	2049	N	PHE	A	282	-5.800	7.237	-2.763	1.00	41.21
AAAA										
ATOM	2050	CA	PHE	A	282	-7.206	6.887	-2.910	1.00	44.31
AAAA										
ATOM	2051	CB	PHE	A	282	-7.722	6.169	-1.664	1.00	45.63
AAAA										
ATOM	2052	CG	PHE	A	282	-9.142	5.697	-1.785	1.00	47.68
AAAA										
ATOM	2053	CD1	PHE	A	282	-9.452	4.570	-2.542	1.00	48.21
AAAA										
ATOM	2054	CD2	PHE	A	282	-10.176	6.387	-1.156	1.00	48.55
AAAA										
ATOM	2055	CE1	PHE	A	282	-10.772	4.136	-2.673	1.00	49.11
AAAA										
ATOM	2056	CE2	PHE	A	282	-11.501	5.963	-1.280	1.00	49.07
AAAA										
ATOM	2057	CZ	PHE	A	282	-11.799	4.833	-2.041	1.00	48.80
AAAA										
ATOM	2058	C	PHE	A	282	-7.908	8.233	-3.052	1.00	45.26
AAAA										
ATOM	2059	O	PHE	A	282	-7.720	9.121	-2.224	1.00	45.48
AAAA										
ATOM	2060	N	GLN	A	283	-8.706	8.387	-4.101	1.00	47.00
AAAA										
ATOM	2061	CA	GLN	A	283	-9.399	9.648	-4.339	1.00	48.78
AAAA										
ATOM	2062	CB	GLN	A	283	-9.958	9.677	-5.768	1.00	48.98
AAAA										
ATOM	2063	CG	GLN	A	283	-10.606	11.000	-6.170	1.00	50.07
AAAA										
ATOM	2064	CD	GLN	A	283	-9.649	12.179	-6.082	1.00	50.05
AAAA										
ATOM	2065	OE1	GLN	A	283	-9.206	12.556	-4.997	1.00	50.12
AAAA										
ATOM	2066	NE2	GLN	A	283	-9.321	12.762	-7.230	1.00	50.62
AAAA										
ATOM	2067	C	GLN	A	283	-10.519	9.918	-3.335	1.00	49.60
AAAA										
ATOM	2068	O	GLN	A	283	-11.317	9.035	-3.018	1.00	49.68
AAAA										
ATOM	2069	N	HIS	A	284	-10.558	11.151	-2.838	1.00	50.76
AAAA										
ATOM	2070	CA	HIS	A	284	-11.570	11.579	-1.875	1.00	51.60
AAAA										
ATOM	2071	CB	HIS	A	284	-11.329	10.918	-0.515	1.00	52.12
AAAA										

ATOM AAAA	2072	CG	HIS	A	284	-12.436	11.140	0.469	1.00 52.63
ATOM AAAA	2073	CD2	HIS	A	284	-13.327	10.280	1.017	1.00 52.98
ATOM AAAA	2074	ND1	HIS	A	284	-12.733	12.381	0.991	1.00 52.98
ATOM AAAA	2075	CE1	HIS	A	284	-13.758	12.276	1.817	1.00 52.69
ATOM AAAA	2076	NE2	HIS	A	284	-14.138	11.011	1.851	1.00 52.96
ATOM AAAA	2077	C	HIS	A	284	-11.497	13.098	-1.745	1.00 52.04
ATOM AAAA	2078	O	HIS	A	284	-10.451	13.697	-2.000	1.00 52.03
ATOM AAAA	2079	N	LYS	A	285	-12.604	13.719	-1.347	1.00 52.27
ATOM AAAA	2080	CA	LYS	A	285	-12.653	15.171	-1.210	1.00 52.70
ATOM AAAA	2081	CB	LYS	A	285	-14.018	15.604	-0.669	1.00 53.61
ATOM AAAA	2082	CG	LYS	A	285	-14.256	17.111	-0.701	1.00 55.17
ATOM AAAA	2083	CD	LYS	A	285	-14.503	17.634	-2.122	1.00 56.00
ATOM AAAA	2084	CE	LYS	A	285	-13.244	17.625	-2.984	1.00 56.62
ATOM AAAA	2085	NZ	LYS	A	285	-13.513	18.075	-4.383	1.00 56.60
ATOM AAAA	2086	C	LYS	A	285	-11.552	15.746	-0.319	1.00 52.35
ATOM AAAA	2087	O	LYS	A	285	-10.988	16.800	-0.619	1.00 51.96
ATOM AAAA	2088	N	ASP	A	286	-11.246	15.054	0.773	1.00 51.71
ATOM AAAA	2089	CA	ASP	A	286	-10.218	15.521	1.693	1.00 51.34
ATOM AAAA	2090	CB	ASP	A	286	-10.405	14.869	3.067	1.00 53.33
ATOM AAAA	2091	CG	ASP	A	286	-10.003	13.403	3.083	1.00 55.00
ATOM AAAA	2092	OD1	ASP	A	286	-10.412	12.648	2.174	1.00 56.57
ATOM AAAA	2093	OD2	ASP	A	286	-9.280	13.004	4.018	1.00 56.62
ATOM AAAA	2094	C	ASP	A	286	-8.817	15.230	1.164	1.00 49.69
ATOM AAAA	2095	O	ASP	A	286	-7.840	15.829	1.616	1.00 49.71
ATOM AAAA	2096	N	ARG	A	287	-8.724	14.315	0.203	1.00 47.93
ATOM AAAA	2097	CA	ARG	A	287	-7.436	13.944	-0.380	1.00 45.79
ATOM AAAA	2098	CB	ARG	A	287	-6.848	15.121	-1.156	1.00 45.56
ATOM AAAA	2099	CG	ARG	A	287	-7.744	15.660	-2.251	1.00 45.87
ATOM AAAA	2100	CD	ARG	A	287	-7.172	16.949	-2.801	1.00 45.75
ATOM AAAA	2101	NE	ARG	A	287	-5.999	16.724	-3.637	1.00 46.20
ATOM AAAA	2102	CZ	ARG	A	287	-4.981	17.573	-3.733	1.00 46.22
ATOM AAAA	2103	NH1	ARG	A	287	-4.986	18.702	-3.037	1.00 46.26
ATOM AAAA	2104	NH2	ARG	A	287	-3.962	17.297	-4.533	1.00 46.42

ATOM AAAA	2105	C	ARG	A	287	-6.464	13.533	0.722	1.00 44.13
ATOM AAAA	2106	O	ARG	A	287	-5.279	13.870	0.685	1.00 43.87
ATOM AAAA	2107	N	GLN	A	288	-6.975	12.804	1.704	1.00 42.92
ATOM AAAA	2108	CA	GLN	A	288	-6.157	12.359	2.824	1.00 42.41
ATOM AAAA	2109	CB	GLN	A	288	-6.955	11.395	3.704	1.00 42.02
ATOM AAAA	2110	CG	GLN	A	288	-6.226	10.947	4.958	1.00 41.95
ATOM AAAA	2111	CD	GLN	A	288	-7.033	9.951	5.766	1.00 42.04
ATOM AAAA	2112	OE1	GLN	A	288	-7.356	8.860	5.288	1.00 41.14
ATOM AAAA	2113	NE2	GLN	A	288	-7.369	10.322	6.997	1.00 41.32
ATOM AAAA	2114	C	GLN	A	288	-4.867	11.682	2.372	1.00 41.36
ATOM AAAA	2115	O	GLN	A	288	-3.772	12.113	2.734	1.00 41.61
ATOM AAAA	2116	N	GLN	A	289	-4.999	10.626	1.575	1.00 41.32
ATOM AAAA	2117	CA	GLN	A	289	-3.835	9.886	1.105	1.00 40.21
ATOM AAAA	2118	CB	GLN	A	289	-4.267	8.678	0.280	1.00 39.57
ATOM AAAA	2119	CG	GLN	A	289	-5.126	7.703	1.068	1.00 37.69
ATOM AAAA	2120	CD	GLN	A	289	-4.976	6.274	0.595	1.00 37.80
ATOM AAAA	2121	OE1	GLN	A	289	-4.422	6.014	-0.475	1.00 35.48
ATOM AAAA	2122	NE2	GLN	A	289	-5.478	5.337	1.388	1.00 36.57
ATOM AAAA	2123	C	GLN	A	289	-2.862	10.744	0.318	1.00 40.38
ATOM AAAA	2124	O	GLN	A	289	-1.661	10.469	0.301	1.00 40.11
ATOM AAAA	2125	N	TYR	A	290	-3.373	11.782	-0.335	1.00 40.27
ATOM AAAA	2126	CA	TYR	A	290	-2.504	12.678	-1.081	1.00 39.93
ATOM AAAA	2127	CB	TYR	A	290	-3.316	13.715	-1.860	1.00 41.72
ATOM AAAA	2128	CG	TYR	A	290	-2.473	14.873	-2.352	1.00 43.41
ATOM AAAA	2129	CD1	TYR	A	290	-1.590	14.716	-3.421	1.00 44.44
ATOM AAAA	2130	CE1	TYR	A	290	-0.764	15.763	-3.836	1.00 45.65
ATOM AAAA	2131	CD2	TYR	A	290	-2.513	16.109	-1.709	1.00 43.91
ATOM AAAA	2132	CE2	TYR	A	290	-1.695	17.161	-2.111	1.00 45.19
ATOM AAAA	2133	CZ	TYR	A	290	-0.821	16.981	-3.174	1.00 46.54
ATOM AAAA	2134	OH	TYR	A	290	0.003	18.014	-3.566	1.00 47.98
ATOM AAAA	2135	C	TYR	A	290	-1.604	13.399	-0.085	1.00 39.33
ATOM AAAA	2136	O	TYR	A	290	-0.396	13.529	-0.296	1.00 39.19
ATOM AAAA	2137	N	TRP	A	291	-2.202	13.871	1.005	1.00 38.32

ATOM	2138	CA	TRP	A	291	-1.451	14.585	2.025	1.00 37.84
AAAA									
ATOM	2139	CB	TRP	A	291	-2.409	15.307	2.979	1.00 37.98
AAAA									
ATOM	2140	CG	TRP	A	291	-3.211	16.366	2.286	1.00 39.40
AAAA									
ATOM	2141	CD2	TRP	A	291	-2.721	17.612	1.778	1.00 39.83
AAAA									
ATOM	2142	CE2	TRP	A	291	-3.810	18.270	1.162	1.00 40.18
AAAA									
ATOM	2143	CE3	TRP	A	291	-1.467	18.238	1.781	1.00 40.07
AAAA									
ATOM	2144	CD1	TRP	A	291	-4.540	16.319	1.969	1.00 38.96
AAAA									
ATOM	2145	NE1	TRP	A	291	-4.908	17.459	1.294	1.00 39.51
AAAA									
ATOM	2146	CZ2	TRP	A	291	-3.684	19.525	0.554	1.00 40.53
AAAA									
ATOM	2147	CZ3	TRP	A	291	-1.340	19.488	1.177	1.00 41.40
AAAA									
ATOM	2148	CH2	TRP	A	291	-2.446	20.116	0.572	1.00 40.92
AAAA									
ATOM	2149	C	TRP	A	291	-0.506	13.680	2.803	1.00 36.79
AAAA									
ATOM	2150	O	TRP	A	291	0.515	14.141	3.306	1.00 36.64
AAAA									
ATOM	2151	N	ASN	A	292	-0.841	12.397	2.907	1.00 36.82
AAAA									
ATOM	2152	CA	ASN	A	292	0.030	11.467	3.619	1.00 37.08
AAAA									
ATOM	2153	CB	ASN	A	292	-0.658	10.116	3.842	1.00 36.47
AAAA									
ATOM	2154	CG	ASN	A	292	-1.841	10.203	4.783	1.00 36.02
AAAA									
ATOM	2155	OD1	ASN	A	292	-1.924	11.104	5.618	1.00 35.88
AAAA									
ATOM	2156	ND2	ASN	A	292	-2.757	9.248	4.667	1.00 35.26
AAAA									
ATOM	2157	C	ASN	A	292	1.302	11.246	2.803	1.00 37.41
AAAA									
ATOM	2158	O	ASN	A	292	2.402	11.170	3.353	1.00 36.90
AAAA									
ATOM	2159	N	ALA	A	293	1.138	11.166	1.485	1.00 38.20
AAAA									
ATOM	2160	CA	ALA	A	293	2.253	10.936	0.567	1.00 38.64
AAAA									
ATOM	2161	CB	ALA	A	293	1.729	10.343	-0.737	1.00 37.83
AAAA									
ATOM	2162	C	ALA	A	293	3.085	12.176	0.267	1.00 39.51
AAAA									
ATOM	2163	O	ALA	A	293	4.311	12.094	0.158	1.00 39.51
AAAA									
ATOM	2164	N	LEU	A	294	2.422	13.321	0.137	1.00 40.40
AAAA									
ATOM	2165	CA	LEU	A	294	3.101	14.575	-0.169	1.00 40.96
AAAA									
ATOM	2166	CB	LEU	A	294	2.166	15.757	0.101	1.00 41.41
AAAA									
ATOM	2167	CG	LEU	A	294	2.666	17.155	-0.272	1.00 41.36
AAAA									
ATOM	2168	CD1	LEU	A	294	3.231	17.168	-1.688	1.00 41.61
AAAA									
ATOM	2169	CD2	LEU	A	294	1.510	18.136	-0.147	1.00 41.60
AAAA									
ATOM	2170	C	LEU	A	294	4.419	14.762	0.585	1.00 42.04
AAAA									

ATOM 2171 O LEU A 294 5.404 15.228 0.013 1.00 42.14
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ATOM 2172 N PRO A 295 4.459 14.401 1.877 1.00 42.80
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ATOM 2173 CD PRO A 295 3.351 14.022 2.772 1.00 42.95
AAAA
ATOM 2174 CA PRO A 295 5.706 14.560 2.634 1.00 43.42
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ATOM 2175 CB PRO A 295 5.336 14.032 4.015 1.00 43.51
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ATOM 2177 C PRO A 295 6.900 13.813 2.022 1.00 44.05
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ATOM 2179 N LEU A 296 6.682 12.577 1.581 1.00 44.41
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ATOM 2182 CG LEU A 296 7.424 9.484 2.130 1.00 44.46
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ATOM 2188 CA GLU A 297 7.421 13.291 -2.502 1.00 47.94
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ATOM 2189 CB GLU A 297 6.113 13.563 -3.251 1.00 48.43
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ATOM 2190 CG GLU A 297 6.306 14.349 -4.544 1.00 49.91
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ATOM 2191 CD GLU A 297 5.014 14.543 -5.318 1.00 51.34
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ATOM 2192 OE1 GLU A 297 4.562 13.586 -5.981 1.00 51.89
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ATOM 2193 OE2 GLU A 297 4.446 15.655 -5.257 1.00 52.41
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ATOM 2194 C GLU A 297 8.225 14.579 -2.393 1.00 48.46
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ATOM 2196 N LYS A 298 7.860 15.421 -1.431 1.00 49.07
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ATOM 2197 CA LYS A 298 8.556 16.685 -1.226 1.00 49.76
AAAA
ATOM 2198 CB LYS A 298 7.914 17.468 -0.077 1.00 50.85
AAAA
ATOM 2199 CG LYS A 298 8.644 18.753 0.277 1.00 52.14
AAAA
ATOM 2200 CD LYS A 298 8.032 19.429 1.492 1.00 53.44
AAAA
ATOM 2201 CE LYS A 298 8.820 20.675 1.882 1.00 53.80
AAAA
ATOM 2202 NZ LYS A 298 8.281 21.309 3.116 1.00 54.32
AAAA
ATOM 2203 C LYS A 298 10.022 16.420 -0.908 1.00 49.36
AAAA

ATOM	2204	O	LYS	A	298	10.904	17.180	-1.305	1.00	50.01
AAAA										
ATOM	2205	N	ALA	A	299	10.275	15.335	-0.188	1.00	48.67
AAAA										
ATOM	2206	CA	ALA	A	299	11.635	14.975	0.182	1.00	47.48
AAAA										
ATOM	2207	CB	ALA	A	299	11.615	14.001	1.353	1.00	47.29
AAAA										
ATOM	2208	C	ALA	A	299	12.354	14.356	-1.009	1.00	46.69
AAAA										
ATOM	2209	O	ALA	A	299	13.554	14.098	-0.953	1.00	46.67
AAAA										
ATOM	2210	N	GLY	A	300	11.613	14.133	-2.090	1.00	45.80
AAAA										
ATOM	2211	CA	GLY	A	300	12.197	13.538	-3.278	1.00	44.79
AAAA										
ATOM	2212	C	GLY	A	300	12.399	12.042	-3.119	1.00	44.04
AAAA										
ATOM	2213	O	GLY	A	300	13.343	11.472	-3.665	1.00	44.02
AAAA										
ATOM	2214	N	ALA	A	301	11.505	11.404	-2.370	1.00	43.01
AAAA										
ATOM	2215	CA	ALA	A	301	11.589	9.967	-2.131	1.00	42.10
AAAA										
ATOM	2216	CB	ALA	A	301	11.514	9.684	-0.632	1.00	42.10
AAAA										
ATOM	2217	C	ALA	A	301	10.484	9.209	-2.858	1.00	41.88
AAAA										
ATOM	2218	O	ALA	A	301	10.480	7.976	-2.882	1.00	41.48
AAAA										
ATOM	2219	N	ALA	A	302	9.549	9.941	-3.453	1.00	40.88
AAAA										
ATOM	2220	CA	ALA	A	302	8.451	9.303	-4.156	1.00	40.59
AAAA										
ATOM	2221	CB	ALA	A	302	7.411	8.818	-3.153	1.00	39.61
AAAA										
ATOM	2222	C	ALA	A	302	7.786	10.197	-5.191	1.00	40.72
AAAA										
ATOM	2223	O	ALA	A	302	8.123	11.372	-5.340	1.00	40.90
AAAA										
ATOM	2224	N	LYS	A	303	6.837	9.610	-5.910	1.00	41.39
AAAA										
ATOM	2225	CA	LYS	A	303	6.073	10.309	-6.930	1.00	41.79
AAAA										
ATOM	2226	CB	LYS	A	303	6.455	9.807	-8.325	1.00	41.86
AAAA										
ATOM	2227	CG	LYS	A	303	5.540	10.295	-9.442	1.00	43.46
AAAA										
ATOM	2228	CD	LYS	A	303	5.608	11.807	-9.614	1.00	44.98
AAAA										
ATOM	2229	CE	LYS	A	303	4.676	12.284	-10.729	1.00	46.33
AAAA										
ATOM	2230	NZ	LYS	A	303	4.767	13.759	-10.957	1.00	46.15
AAAA										
ATOM	2231	C	LYS	A	303	4.603	10.022	-6.671	1.00	41.86
AAAA										
ATOM	2232	O	LYS	A	303	4.219	8.873	-6.441	1.00	41.54
AAAA										
ATOM	2233	N	ILE	A	304	3.782	11.065	-6.702	1.00	41.98
AAAA										
ATOM	2234	CA	ILE	A	304	2.354	10.905	-6.475	1.00	42.52
AAAA										
ATOM	2235	CB	ILE	A	304	1.808	11.961	-5.492	1.00	42.27
AAAA										
ATOM	2236	CG2	ILE	A	304	0.321	11.738	-5.278	1.00	41.77
AAAA										

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ATOM   2237  CG1 ILE A 304       2.554  11.889  -4.159  1.00 42.76
AAAA
ATOM   2238  CD1 ILE A 304       2.094  12.921  -3.140  1.00 41.84
AAAA
ATOM   2239  C   ILE A 304       1.580  11.047  -7.777  1.00 43.43
AAAA
ATOM   2240  O   ILE A 304       1.818  11.969  -8.555  1.00 43.89
AAAA
ATOM   2241  N   ILE A 305       0.649  10.129  -8.006  1.00 44.38
AAAA
ATOM   2242  CA  ILE A 305      -0.177  10.164  -9.199  1.00 45.28
AAAA
ATOM   2243  CB  ILE A 305       0.287   9.124 -10.247  1.00 44.81
AAAA
ATOM   2244  CG2 ILE A 305      -0.610   9.188 -11.478  1.00 43.86
AAAA
ATOM   2245  CG1 ILE A 305       1.738   9.400 -10.647  1.00 44.38
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ATOM   2246  CD1 ILE A 305       2.305   8.405 -11.647  1.00 45.12
AAAA
ATOM   2247  C   ILE A 305      -1.620   9.870  -8.807  1.00 47.13
AAAA
ATOM   2248  O   ILE A 305      -1.985   8.724  -8.550  1.00 46.47
AAAA                                                    /
ATOM   2249  N   GLU A 306      -2.435  10.918  -8.745  1.00 49.50
AAAA
ATOM   2250  CA  GLU A 306      -3.839  10.761  -8.396  1.00 51.69
AAAA
ATOM   2251  CB  GLU A 306      -4.430  12.110  -7.987  1.00 51.85
AAAA
ATOM   2252  CG  GLU A 306      -3.603  12.818  -6.927  1.00 51.67
AAAA
ATOM   2253  CD  GLU A 306      -4.324  13.990  -6.296  1.00 52.25
AAAA
ATOM   2254  OE1 GLU A 306      -5.351  13.763  -5.621  1.00 52.52
AAAAATOM   2255  OE2 GLU A 306      -3.861  15.135  -6.472  1.00 52.12
AAAAATOM   2256  C   GLU A 306      -4.552  10.202  -9.619  1.00 53.21
AAAAATOM   2257  O   GLU A 306      -4.180  10.515 -10.749  1.00 53.53
AAAAATOM   2258  N   GLN A 307      -5.570   9.376  -9.393  1.00 55.39
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AAAAATOM   2260  CB  GLN A 307      -7.553   8.035  -9.934  1.00 58.22
AAAAATOM   2261  CG  GLN A 307      -7.213   6.925  -8.937  1.00 59.17
AAAAATOM   2262  CD  GLN A 307      -8.196   5.766  -8.970  1.00 59.83
AAAAATOM   2263  OE1 GLN A 307      -8.110   4.840  -8.160  1.00 60.26
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AAAAATOM   2268  CD  PRO A 308      -7.113  11.674 -10.105  1.00 59.76
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AAAAATOM   2274  N   GLN A 309      -5.042  11.881 -13.305  1.00 59.45
AAAAATOM   2275  CA  GLN A 309      -3.985  11.794 -14.303  1.00 58.69
AAAAATOM   2276  CB  GLN A 309      -2.992  12.947 -14.135  1.00 59.92
AAAAATOM   2277  CG  GLN A 309      -2.082  12.838 -12.920  1.00 60.97
AAAAATOM   2278  CD  GLN A 309      -1.077  13.975 -12.843  1.00 61.96
AAAAATOM   2279  OE1 GLN A 309      -0.180  13.974 -11.997  1.00 62.79
AAAAATOM   2280  NE2 GLN A 309      -1.226  14.956 -13.728  1.00 62.49
AAAAATOM   2281  C   GLN A 309      -3.250  10.459 -14.204  1.00 57.53
AAAAATOM   2282  O   GLN A 309      -2.078  10.358 -14.567  1.00 57.67
AAAAATOM   2283  N   LEU A 310      -3.947   9.437 -13.711  1.00 55.75
AAAAATOM   2284  CA  LEU A 310      -3.364   8.107 -13.570  1.00 53.92
AAAAATOM   2285  CB  LEU A 310      -3.799   7.473 -12.241  1.00 53.77
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AAAAATOM	2286	CG	LEU	A	310	-3.242	6.108	-11.804	1.00	53.75
AAAAATOM	2287	CD1	LEU	A	310	-3.810	4.998	-12.669	1.00	54.14
AAAAATOM	2288	CD2	LEU	A	310	-1.727	6.123	-11.876	1.00	52.88
AAAAATOM	2289	C	LEU	A	310	-3.813	7.243	-14.740	1.00	52.48
AAAAATOM	2290	O	LEU	A	310	-5.003	7.162	-15.044	1.00	53.10
AAAAATOM	2291	N	SER	A	311	-2.852	6.603	-15.395	1.00	49.96
AAAAATOM	2292	CA	SER	A	311	-3.136	5.748	-16.540	1.00	47.96
AAAAATOM	2293	CB	SER	A	311	-3.409	6.599	-17.778	1.00	47.62
AAAAATOM	2294	OG	SER	A	311	-2.232	7.287	-18.168	1.00	46.72
AAAAATOM	2295	C	SER	A	311	-1.936	4.849	-16.815	1.00	46.16
AAAAATOM	2296	O	SER	A	311	-0.873	5.018	-16.212	1.00	45.34
AAAAATOM	2297	N	VAL	A	312	-2.113	3.907	-17.736	1.00	44.77
AAAAATOM	2298	CA	VAL	A	312	-1.056	2.972	-18.103	1.00	43.52
AAAAATOM	2299	CB	VAL	A	312	-1.496	2.066	-19.278	1.00	43.96
AAAAATOM	2300	CG1	VAL	A	312	-0.373	1.112	-19.656	1.00	43.81
AAAAATOM	2301	CG2	VAL	A	312	-2.740	1.285	-18.892	1.00	43.95
AAAAATOM	2302	C	VAL	A	312	0.215	3.712	-18.498	1.00	42.79
AAAAATOM	2303	O	VAL	A	312	1.284	3.488	-17.922	1.00	41.92
AAAAATOM	2304	N	ASP	A	313	0.096	4.610	-19.470	1.00	42.00
AAAAATOM	2305	CA	ASP	A	313	1.252	5.364	-19.939	1.00	41.37
AAAAATOM	2306	CB	ASP	A	313	0.877	6.203	-21.163	1.00	43.96
AAAAATOM	2307	CG	ASP	A	313	0.506	5.345	-22.357	1.00	46.32
AAAAATOM	2308	OD1	ASP	A	313	1.334	4.496	-22.755	1.00	47.81
AAAAATOM	2309	OD2	ASP	A	313	-0.610	5.514	-22.896	1.00	48.38
AAAAATOM	2310	C	ASP	A	313	1.856	6.249	-18.864	1.00	39.53
AAAAATOM	2311	O	ASP	A	313	3.069	6.452	-18.832	1.00	39.95
AAAAATOM	2312	N	ALA	A	314	1.015	6.768	-17.978	1.00	38.08
AAAAATOM	2313	CA	ALA	A	314	1.492	7.629	-16.905	1.00	36.44
AAAAATOM	2314	CB	ALA	A	314	0.306	8.233	-16.156	1.00	36.79
AAAAATOM	2315	C	ALA	A	314	2.382	6.844	-15.939	1.00	35.41
AAAAATOM	2316	O	ALA	A	314	3.448	7.313	-15.535	1.00	35.44
AAAAATOM	2317	N	VAL	A	315	1.940	5.648	-15.569	1.00	34.29
AAAAATOM	2318	CA	VAL	A	315	2.708	4.809	-14.652	1.00	33.44
AAAAATOM	2319	CB	VAL	A	315	1.886	3.592	-14.169	1.00	33.40
AAAAATOM	2320	CG1	VAL	A	315	2.707	2.775	-13.180	1.00	33.12
AAAAATOM	2321	CG2	VAL	A	315	0.588	4.059	-13.521	1.00	32.76
AAAAATOM	2322	C	VAL	A	315	3.970	4.295	-15.328	1.00	32.88
AAAAATOM	2323	O	VAL	A	315	5.071	4.426	-14.792	1.00	32.35
AAAAATOM	2324	N	ALA	A	316	3.805	3.708	-16.508	1.00	33.02
AAAAATOM	2325	CA	ALA	A	316	4.940	3.172	-17.250	1.00	34.17
AAAAATOM	2326	CB	ALA	A	316	4.469	2.616	-18.593	1.00	33.68
AAAAATOM	2327	C	ALA	A	316	6.002	4.252	-17.456	1.00	34.75
AAAAATOM	2328	O	ALA	A	316	7.190	4.026	-17.211	1.00	34.70
AAAAATOM	2329	N	ASN	A	317	5.578	5.434	-17.889	1.00	35.49
AAAAATOM	2330	CA	ASN	A	317	6.524	6.518	-18.108	1.00	35.27
AAAAATOM	2331	CB	ASN	A	317	5.815	7.738	-18.694	1.00	37.74
AAAAATOM	2332	CG	ASN	A	317	5.395	7.518	-20.128	1.00	38.86
AAAAATOM	2333	OD1	ASN	A	317	6.099	6.855	-20.889	1.00	39.80
AAAAATOM	2334	ND2	ASN	A	317	4.252	8.077	-20.511	1.00	40.96
AAAAATOM	2335	C	ASN	A	317	7.272	6.916	-16.847	1.00	35.18
AAAAATOM	2336	O	ASN	A	317	8.458	7.239	-16.904	1.00	34.36
AAAAATOM	2337	N	THR	A	318	6.592	6.891	-15.704	1.00	34.31
AAAAATOM	2338	CA	THR	A	318	7.251	7.262	-14.456	1.00	34.35
AAAAATOM	2339	CB	THR	A	318	6.245	7.358	-13.282	1.00	34.55
AAAAATOM	2340	OG1	THR	A	318	5.353	8.460	-13.498	1.00	34.46
AAAAATOM	2341	CG2	THR	A	318	6.984	7.568	-11.969	1.00	34.42
AAAAATOM	2342	C	THR	A	318	8.335	6.252	-14.093	1.00	34.52
AAAAATOM	2343	O	THR	A	318	9.464	6.624	-13.783	1.00	34.11
AAAAATOM	2344	N	LEU	A	319	7.987	4.971	-14.139	1.00	35.35
AAAAATOM	2345	CA	LEU	A	319	8.937	3.918	-13.801	1.00	35.23
AAAAATOM	2346	CB	LEU	A	319	8.233	2.556	-13.804	1.00	34.91
AAAAATOM	2347	CG	LEU	A	319	7.142	2.362	-12.743	1.00	34.50
AAAAATOM	2348	CD1	LEU	A	319	6.445	1.031	-12.956	1.00	34.48
AAAAATOM	2349	CD2	LEU	A	319	7.761	2.432	-11.351	1.00	35.13
AAAAATOM	2350	C	LEU	A	319	10.107	3.907	-14.777	1.00	35.72
AAAAATOM	2351	O	LEU	A	319	11.264	3.830	-14.370	1.00	34.85

AAAAATOM	2352	N	ALA	A	320	9.801	3.997	-16.067	1.00	36.49
AAAAATOM	2353	CA	ALA	A	320	10.832	3.989	-17.096	1.00	38.10
AAAAATOM	2354	CB	ALA	A	320	10.192	4.051	-18.472	1.00	37.58
AAAAATOM	2355	C	ALA	A	320	11.809	5.144	-16.924	1.00	38.94
AAAAATOM	2356	O	ALA	A	320	12.939	5.087	-17.410	1.00	39.51
AAAAATOM	2357	N	GLY	A	321	11.375	6.186	-16.219	1.00	38.88
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AAAAATOM	2359	C	GLY	A	321	13.117	7.303	-14.788	1.00	38.70
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AAAAATOM	2361	N	TRP	A	322	13.028	6.230	-14.010	1.00	38.46
AAAAATOM	2362	CA	TRP	A	322	13.855	6.108	-12.820	1.00	38.53
AAAAATOM	2363	CB	TRP	A	322	13.008	5.688	-11.611	1.00	39.41
AAAAATOM	2364	CG	TRP	A	322	12.047	6.748	-11.146	1.00	40.01
AAAAATOM	2365	CD2	TRP	A	322	10.898	6.558	-10.307	1.00	40.49
AAAAATOM	2366	CE2	TRP	A	322	10.330	7.833	-10.081	1.00	41.27
AAAAATOM	2367	CE3	TRP	A	322	10.295	5.436	-9.722	1.00	40.54
AAAAATOM	2368	CD1	TRP	A	322	12.126	8.091	-11.389	1.00	39.97
AAAAATOM	2369	NE1	TRP	A	322	11.098	8.749	-10.752	1.00	40.69
AAAAATOM	2370	CZ2	TRP	A	322	9.186	8.018	-9.293	1.00	41.67
AAAAATOM	2371	CZ3	TRP	A	322	9.155	5.619	-8.938	1.00	41.40
AAAAATOM	2372	CH2	TRP	A	322	8.615	6.903	-8.732	1.00	41.69
AAAAATOM	2373	C	TRP	A	322	14.984	5.109	-13.027	1.00	38.48
AAAAATOM	2374	O	TRP	A	322	14.743	3.929	-13.271	1.00	38.22
AAAAATOM	2375	N	SER	A	323	16.217	5.596	-12.935	1.00	38.13
AAAAATOM	2376	CA	SER	A	323	17.395	4.753	-13.101	1.00	38.51
AAAAATOM	2377	CB	SER	A	323	18.573	5.590	-13.591	1.00	38.51
AAAAATOM	2378	OG	SER	A	323	18.994	6.489	-12.582	1.00	39.52
AAAAATOM	2379	C	SER	A	323	17.739	4.150	-11.744	1.00	38.37
AAAAATOM	2380	O	SER	A	323	17.188	4.566	-10.725	1.00	37.29
AAAAATOM	2381	N	ARG	A	324	18.647	3.178	-11.723	1.00	37.86
AAAAATOM	2382	CA	ARG	A	324	19.030	2.563	-10.461	1.00	37.82
AAAAATOM	2383	CB	ARG	A	324	19.924	1.341	-10.688	1.00	36.36
AAAAATOM	2384	CG	ARG	A	324	19.130	0.077	-10.959	1.00	34.77
AAAAATOM	2385	CD	ARG	A	324	19.978	-1.176	-10.849	1.00	33.04
AAAAATOM	2386	NE	ARG	A	324	19.143	-2.372	-10.888	1.00	31.23
AAAAATOM	2387	CZ	ARG	A	324	18.318	-2.738	-9.908	1.00	29.95
AAAAATOM	2388	NH1	ARG	A	324	18.228	-2.006	-8.808	1.00	28.46
AAAAATOM	2389	NH2	ARG	A	324	17.562	-3.815	-10.041	1.00	28.17
AAAAATOM	2390	C	ARG	A	324	19.731	3.571	-9.569	1.00	38.78
AAAAATOM	2391	O	ARG	A	324	19.532	3.578	-8.354	1.00	38.12
AAAAATOM	2392	N	GLU	A	325	20.551	4.428	-10.169	1.00	39.55
AAAAATOM	2393	CA	GLU	A	325	21.251	5.447	-9.401	1.00	40.60
AAAAATOM	2394	CB	GLU	A	325	22.208	6.236	-10.304	1.00	42.74
AAAAATOM	2395	CG	GLU	A	325	22.642	7.589	-9.745	1.00	46.19
AAAAATOM	2396	CD	GLU	A	325	23.197	7.517	-8.327	1.00	48.10
AAAAATOM	2397	OE1	GLU	A	325	23.535	8.586	-7.770	1.00	49.61
AAAAATOM	2398	OE2	GLU	A	325	23.297	6.403	-7.768	1.00	49.87
AAAAATOM	2399	C	GLU	A	325	20.214	6.380	-8.784	1.00	39.88
AAAAATOM	2400	O	GLU	A	325	20.324	6.771	-7.623	1.00	39.45
AAAAATOM	2401	N	THR	A	326	19.202	6.725	-9.572	1.00	39.89
AAAAATOM	2402	CA	THR	A	326	18.130	7.591	-9.102	1.00	40.25
AAAAATOM	2403	CB	THR	A	326	17.139	7.912	-10.240	1.00	40.72
AAAAATOM	2404	OG1	THR	A	326	17.828	8.593	-11.298	1.00	42.28
AAAAATOM	2405	CG2	THR	A	326	16.006	8.795	-9.730	1.00	41.64
AAAAATOM	2406	C	THR	A	326	17.371	6.897	-7.968	1.00	39.76
AAAAATOM	2407	O	THR	A	326	17.108	7.497	-6.925	1.00	39.87
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AAAAATOM	2409	CA	LEU	A	327	16.294	4.867	-7.169	1.00	37.41
AAAAATOM	2410	CB	LEU	A	327	15.968	3.466	-7.697	1.00	36.19
AAAAATOM	2411	CG	LEU	A	327	14.952	3.426	-8.843	1.00	35.32
AAAAATOM	2412	CD1	LEU	A	327	14.802	2.002	-9.370	1.00	35.07
AAAAATOM	2413	CD2	LEU	A	327	13.614	3.961	-8.354	1.00	34.69
AAAAATOM	2414	C	LEU	A	327	17.050	4.774	-5.845	1.00	37.39
AAAAATOM	2415	O	LEU	A	327	16.437	4.807	-4.778	1.00	36.80
AAAAATOM	2416	N	LEU	A	328	18.375	4.665	-5.909	1.00	37.58
AAAAATOM	2417	CA	LEU	A	328	19.184	4.593	-4.693	1.00	38.35

AAAAATOM	2418	CB	LEU	A	328	20.662	4.368	-5.030	1.00	38.95
AAAAATOM	2419	CG	LEU	A	328	21.636	3.544	-3.854	1.00	40.10
AAAAATOM	2420	CD1	LEU	A	328	21.303	3.551	-2.752	1.00	39.51
AAAAATOM	2421	CD2	LEU	A	328	23.068	4.349	-4.330	1.00	40.30
AAAAATOM	2422	C	LEU	A	328	19.039	5.899	-3.926	1.00	38.68
AAAAATOM	2423	O	LEU	A	328	18.929	5.906	-2.697	1.00	38.65
AAAAATOM	2424	N	THR	A	329	19.048	7.004	-4.664	1.00	39.35
AAAAATOM	2425	CA	THR	A	329	18.908	8.326	-4.068	1.00	39.98
AAAAATOM	2426	CB	THR	A	329	19.002	9.433	-5.136	1.00	40.05
AAAAATOM	2427	OG1	THR	A	329	20.280	9.364	-5.782	1.00	41.54
AAAAATOM	2428	CG2	THR	A	329	18.841	10.808	-4.497	1.00	40.35
AAAAATOM	2429	C	THR	A	329	17.557	8.425	-3.367	1.00	39.68
AAAAATOM	2430	O	THR	A	329	17.485	8.743	-2.179	1.00	39.91
AAAAATOM	2431	N	MET	A	330	16.492	8.147	-4.111	1.00	39.51
AAAAATOM	2432	CA	MET	A	330	15.143	8.190	-3.564	1.00	38.79
AAAAATOM	2433	CB	MET	A	330	14.141	7.718	-4.617	1.00	38.09
AAAAATOM	2434	CG	MET	A	330	14.011	8.657	-5.804	1.00	36.84
AAAAATOM	2435	SD	MET	A	330	12.977	7.980	-7.108	1.00	37.95
AAAAATOM	2436	CE	MET	A	330	11.332	8.342	-6.478	1.00	37.58
AAAAATOM	2437	C	MET	A	330	15.037	7.315	-2.319	1.00	39.71
AAAAATOM	2438	O	MET	A	330	14.418	7.703	-1.326	1.00	39.60
AAAAATOM	2439	N	ALA	A	331	15.646	6.135	-2.381	1.00	39.50
AAAAATOM	2440	CA	ALA	A	331	15.625	5.202	-1.266	1.00	40.36
AAAAATOM	2441	CB	ALA	A	331	16.378	3.928	-1.634	1.00	39.91
AAAAATOM	2442	C	ALA	A	331	16.243	5.843	-0.032	1.00	40.98
AAAAATOM	2443	O	ALA	A	331	15.662	5.805	1.052	1.00	40.34
AAAAATOM	2444	N	GLU	A	332	17.422	6.435	-0.201	1.00	41.85
AAAAATOM	2445	CA	GLU	A	332	18.102	7.087	0.911	1.00	42.77
AAAAATOM	2446	CB	GLU	A	332	19.470	7.607	0.465	1.00	44.04
AAAAATOM	2447	CG	GLU	A	332	20.414	6.500	0.016	1.00	46.55
AAAAATOM	2448	CD	GLU	A	332	21.822	6.994	-0.248	1.00	48.04
AAAAATOM	2449	OE1	GLU	A	332	21.981	7.923	-1.065	1.00	49.87
AAAAATOM	2450	OE2	GLU	A	332	22.770	6.449	0.359	1.00	49.38
AAAAATOM	2451	C	GLU	A	332	17.246	8.228	1.445	1.00	42.38
AAAAATOM	2452	O	GLU	A	332	17.156	8.435	2.653	1.00	42.66
AAAAATOM	2453	N	ARG	A	333	16.619	8.969	0.540	1.00	41.80
AAAAATOM	2454	CA	ARG	A	333	15.752	10.067	0.937	1.00	42.25
AAAAATOM	2455	CB	ARG	A	333	15.212	10.784	-0.306	1.00	43.43
AAAAATOM	2456	CG	ARG	A	333	16.184	11.793	-0.926	1.00	45.99
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AAAAATOM	2460	NH1	ARG	A	333	18.585	12.814	-2.297	1.00	52.45
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AAAAATOM	2463	O	ARG	A	333	14.275	10.060	2.834	1.00	40.21
AAAAATOM	2464	N	ALA	A	334	13.981	8.435	1.308	1.00	40.03
AAAAATOM	2465	CA	ALA	A	334	12.859	7.825	2.014	1.00	39.84
AAAAATOM	2466	CB	ALA	A	334	12.356	6.612	1.241	1.00	38.43
AAAAATOM	2467	C	ALA	A	334	13.239	7.417	3.435	1.00	40.05
AAAAATOM	2468	O	ALA	A	334	12.493	7.665	4.386	1.00	40.41
AAAAATOM	2469	N	ARG	A	335	14.404	6.797	3.577	1.00	39.11
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AAAAATOM	2476	NH1	ARG	A	335	15.972	1.024	6.274	1.00	43.17
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AAAAATOM	2478	C	ARG	A	335	15.167	7.527	5.802	1.00	40.09
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AAAAATOM	2484	O	ALA	A	336	14.905	11.087	7.621	1.00	42.49
AAAAATOM	2485	N	ALA	A	337	13.725	10.300	5.879	1.00	42.58
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AAAAATOM	2501	CD1	ILE	A	339	9.263	11.423	12.804	1.00	40.42
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AAAAATOM	2514	CG	ASP	A	341	12.044	7.146	18.317	1.00	39.54
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AAAAATOM	2519	N	ALA	A	342	8.329	5.789	16.971	1.00	36.20
AAAAATOM	2520	CA	ALA	A	342	6.996	6.349	17.181	1.00	34.98
AAAAATOM	2521	CB	ALA	A	342	6.150	6.156	15.927	1.00	35.84
AAAAATOM	2522	C	ALA	A	342	6.280	5.744	18.389	1.00	34.17
AAAAATOM	2523	O	ALA	A	342	5.843	6.465	19.289	1.00	33.36
AAAAATOM	2524	N	THR	A	343	6.159	4.421	18.410	1.00	33.49
AAAAATOM	2525	CA	THR	A	343	5.481	3.747	19.512	1.00	33.39
AAAAATOM	2526	CB	THR	A	343	5.567	2.211	19.362	1.00	33.34
AAAAATOM	2527	OG1	THR	A	343	4.951	1.818	18.128	1.00	34.05
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AAAAATOM	2535	CD	GLU	A	344	9.963	2.101	20.581	1.00	44.16
AAAAATOM	2536	OE1	GLU	A	344	10.311	0.917	20.357	1.00	45.57
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AAAAATOM	2538	C	GLU	A	344	7.886	5.856	22.590	1.00	35.95
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BBBBATOM	2669	N	MET	B	10	-3.772	-48.541	-39.604	1.00	27.75
BBBBATOM	2670	CA	MET	B	10	-4.048	-49.055	-38.275	1.00	26.66
BBBBATOM	2671	CB	MET	B	10	-4.268	-50.571	-38.274	1.00	27.09
BBBBATOM	2672	CG	MET	B	10	-4.496	-51.113	-36.869	1.00	28.55
BBBBATOM	2673	SD	MET	B	10	-5.474	-52.612	-36.799	1.00	29.60
BBBBATOM	2674	CE	MET	B	10	-7.126	-51.913	-36.618	1.00	29.41
BBBBATOM	2675	C	MET	B	10	-2.826	-48.691	-37.448	1.00	25.08
BBBBATOM	2676	O	MET	B	10	-1.690	-48.971	-37.839	1.00	24.38
BBBBATOM	2677	N	VAL	B	11	-3.062	-48.037	-36.317	1.00	23.45
BBBBATOM	2678	CA	VAL	B	11	-1.982	-47.605	-35.449	1.00	23.16
BBBBATOM	2679	CB	VAL	B	11	-2.159	-46.116	-35.029	1.00	23.01
BBBBATOM	2680	CG1	VAL	B	11	-0.971	-45.666	-34.184	1.00	20.91
BBBBATOM	2681	CG2	VAL	B	11	-2.305	-45.225	-36.276	1.00	23.82
BBBBATOM	2682	C	VAL	B	11	-1.935	-48.461	-34.184	1.00	23.59
BBBBATOM	2683	O	VAL	B	11	-2.962	-48.712	-33.567	1.00	23.24
BBBBATOM	2684	N	MET	B	12	-0.734	-48.902	-33.817	1.00	23.68
BBBBATOM	2685	CA	MET	B	12	-0.523	-49.707	-32.613	1.00	24.54
BBBBATOM	2686	CB	MET	B	12	0.192	-51.019	-32.971	1.00	24.28
BBBBATOM	2687	CG	MET	B	12	-0.402	-51.726	-34.188	1.00	25.19
BBBBATOM	2688	SD	MET	B	12	0.399	-53.284	-34.669	1.00	26.54
BBBBATOM	2689	CE	MET	B	12	1.990	-52.691	-35.289	1.00	22.99
BBBBATOM	2690	C	MET	B	12	0.361	-48.840	-31.720	1.00	25.31
BBBBATOM	2691	O	MET	B	12	1.546	-48.645	-32.006	1.00	23.88
BBBBATOM	2692	N	ALA	B	13	-0.224	-48.292	-30.657	1.00	27.08
BBBBATOM	2693	CA	ALA	B	13	0.508	-47.410	-29.752	1.00	29.43
BBBBATOM	2694	CB	ALA	B	13	0.747	-46.074	-30.429	1.00	28.82
BBBBATOM	2695	C	ALA	B	13	-0.239	-47.192	-28.436	1.00	31.80
BBBBATOM	2696	O	ALA	B	13	-1.143	-46.350	-28.352	1.00	32.16
BBBBATOM	2697	N	GLY	B	14	0.150	-47.934	-27.405	1.00	32.46
BBBBATOM	2698	CA	GLY	B	14	-0.513	-47.804	-26.120	1.00	33.82
BBBBATOM	2699	C	GLY	B	14	-0.107	-46.595	-25.299	1.00	34.82
BBBBATOM	2700	O	GLY	B	14	0.975	-46.040	-25.479	1.00	35.47
BBBBATOM	2701	N	GLY	B	15	-0.986	-46.188	-24.385	1.00	35.56
BBBBATOM	2702	CA	GLY	B	15	-0.700	-45.047	-23.536	1.00	36.08
BBBBATOM	2703	C	GLY	B	15	0.539	-45.254	-22.683	1.00	36.84
BBBBATOM	2704	O	GLY	B	15	1.293	-44.311	-22.426	1.00	36.03
BBBBATOM	2705	N	THR	B	16	0.755	-46.488	-22.240	1.00	36.65
BBBBATOM	2706	CA	THR	B	16	1.920	-46.787	-21.421	1.00	38.51
BBBBATOM	2707	CB	THR	B	16	1.926	-48.258	-20.974	1.00	38.51
BBBBATOM	2708	OG1	THR	B	16	0.686	-48.558	-20.321	1.00	38.39
BBBBATOM	2709	CG2	THR	B	16	3.075	-48.518	-20.005	1.00	39.11
BBBBATOM	2710	C	THR	B	16	3.158	-46.497	-22.264	1.00	38.35
BBBBATOM	2711	O	THR	B	16	3.191	-46.798	-23.460	1.00	39.90
BBBBATOM	2712	N	GLY	B	17	4.168	-45.897	-21.649	1.00	37.68
BBBBATOM	2713	CA	GLY	B	17	5.367	-45.567	-22.392	1.00	36.57
BBBBATOM	2714	C	GLY	B	17	5.161	-44.303	-23.211	1.00	35.56
BBBBATOM	2715	O	GLY	B	17	6.079	-43.843	-23.890	1.00	35.03
BBBBATOM	2716	N	GLY	B	18	3.949	-43.752	-23.150	1.00	33.83
BBBBATOM	2717	CA	GLY	B	18	3.631	-42.529	-23.872	1.00	33.48
BBBBATOM	2718	C	GLY	B	18	3.825	-42.593	-25.378	1.00	33.12
BBBBATOM	2719	O	GLY	B	18	4.345	-41.650	-25.984	1.00	35.38
BBBBATOM	2720	N	HIS	B	19	3.416	-43.699	-25.988	1.00	30.26
BBBBATOM	2721	CA	HIS	B	19	3.548	-43.865	-27.435	1.00	28.22
BBBBATOM	2722	CB	HIS	B	19	3.772	-45.349	-27.779	1.00	25.81
BBBBATOM	2723	CG	HIS	B	19	4.957	-45.966	-27.094	1.00	25.35
BBBBATOM	2724	CD2	HIS	B	19	6.281	-45.694	-27.184	1.00	24.18
BBBBATOM	2725	ND1	HIS	B	19	4.845	-47.025	-26.217	1.00	24.57
BBBBATOM	2726	CE1	HIS	B	19	6.046	-47.380	-25.798	1.00	23.08
BBBBATOM	2727	NE2	HIS	B	19	6.936	-46.589	-26.369	1.00	25.51
BBBBATOM	2728	C	HIS	B	19	2.280	-43.370	-28.144	1.00	27.91
BBBBATOM	2729	O	HIS	B	19	2.300	-43.049	-29.337	1.00	26.91
BBBBATOM	2730	N	VAL	B	20	1.180	-43.310	-27.402	1.00	27.65
BBBBATOM	2731	CA	VAL	B	20	-0.098	-42.894	-27.965	1.00	27.77
BBBBATOM	2732	CB	VAL	B	20	-1.248	-43.080	-26.942	1.00	28.57

BBBBATOM	2733	CG1	VAL	B	20	-1.082	-42.114	-25.787	1.00	30.03
BBBBATOM	2734	CG2	VAL	B	20	-2.602	-42.873	-27.631	1.00	26.82
BBBBATOM	2735	C	VAL	B	20	-0.140	-41.452	-28.470	1.00	27.57
BBBBATOM	2736	O	VAL	B	20	-0.771	-41.172	-29.486	1.00	27.12
BBBBATOM	2737	N	PHE	B	21	0.528	-40.543	-27.770	1.00	28.03
BBBBATOM	2738	CA	PHE	B	21	0.517	-39.136	-28.160	1.00	29.00
BBBBATOM	2739	CB	PHE	B	21	1.215	-38.289	-27.094	1.00	30.27
BBBBATOM	2740	CG	PHE	B	21	0.565	-38.383	-25.746	1.00	33.59
BBBBATOM	2741	CD1	PHE	B	21	-0.764	-37.999	-25.578	1.00	33.84
BBBBATOM	2742	CD2	PHE	B	21	1.256	-38.909	-24.659	1.00	35.22
BBBBATOM	2743	CE1	PHE	B	21	-1.397	-38.142	-24.350	1.00	35.17
BBBBATOM	2744	CE2	PHE	B	21	0.630	-39.057	-23.422	1.00	36.08
BBBBATOM	2745	CZ	PHE	B	21	-0.700	-38.673	-23.269	1.00	35.65
BBBBATOM	2746	C	PHE	B	21	1.129	-38.898	-29.535	1.00	28.53
BBBBATOM	2747	O	PHE	B	21	0.521	-38.236	-30.378	1.00	28.69
BBBBATOM	2748	N	PRO	B	22	2.336	-39.430	-29.781	1.00	27.41
BBBBATOM	2749	CD	PRO	B	22	3.251	-40.074	-28.819	1.00	27.82
BBBBATOM	2750	CA	PRO	B	22	2.986	-39.252	-31.086	1.00	26.12
BBBBATOM	2751	CB	PRO	B	22	4.362	-39.884	-30.883	1.00	27.48
BBBBATOM	2752	CG	PRO	B	22	4.594	-39.757	-29.403	1.00	28.99
BBBBATOM	2753	C	PRO	B	22	2.188	-39.972	-32.176	1.00	26.37
BBBBATOM	2754	O	PRO	B	22	2.129	-39.522	-33.321	1.00	24.40
BBBBATOM	2755	N	GLY	B	23	1.585	-41.102	-31.807	1.00	24.71
BBBBATOM	2756	CA	GLY	B	23	0.787	-41.864	-32.752	1.00	25.07
BBBBATOM	2757	C	GLY	B	23	-0.459	-41.088	-33.144	1.00	25.00
BBBBATOM	2758	O	GLY	B	23	-0.913	-41.144	-34.295	1.00	23.40
BBBBATOM	2759	N	LEU	B	24	-1.014	-40.366	-32.176	1.00	24.65
BBBBATOM	2760	CA	LEU	B	24	-2.201	-39.551	-32.401	1.00	25.32
BBBBATOM	2761	CB	LEU	B	24	-2.732	-39.017	-31.064	1.00	25.08
BBBBATOM	2762	CG	LEU	B	24	-3.594	-39.997	-30.264	1.00	23.58
BBBBATOM	2763	CD1	LEU	B	24	-3.823	-39.482	-28.828	1.00	25.41
BBBBATOM	2764	CD2	LEU	B	24	-4.919	-40.192	-30.998	1.00	24.78
BBBBATOM	2765	C	LEU	B	24	-1.843	-38.397	-33.336	1.00	25.69
BBBBATOM	2766	O	LEU	B	24	-2.634	-38.017	-34.204	1.00	25.99
BBBBATOM	2767	N	ALA	B	25	-0.644	-37.850	-33.164	1.00	24.89
BBBBATOM	2768	CA	ALA	B	25	-0.197	-36.754	-34.013	1.00	25.94
BBBBATOM	2769	CB	ALA	B	25	1.195	-36.278	-33.590	1.00	25.12
BBBBATOM	2770	C	ALA	B	25	-0.171	-37.207	-35.469	1.00	27.14
BBBBATOM	2771	O	ALA	B	25	-0.626	-36.483	-36.354	1.00	27.46
BBBBATOM	2772	N	VAL	B	26	0.368	-38.403	-35.709	1.00	26.50
BBBBATOM	2773	CA	VAL	B	26	0.466	-38.955	-37.056	1.00	25.70
BBBBATOM	2774	CB	VAL	B	26	1.373	-40.226	-37.081	1.00	26.22
BBBBATOM	2775	CG1	VAL	B	26	1.410	-40.833	-38.479	1.00	26.25
BBBBATOM	2776	CG2	VAL	B	26	2.778	-39.861	-36.631	1.00	24.56
BBBBATOM	2777	C	VAL	B	26	-0.908	-39.310	-37.612	1.00	26.20
BBBBATOM	2778	O	VAL	B	26	-1.178	-39.091	-38.796	1.00	25.87
BBBBATOM	2779	N	ALA	B	27	-1.777	-39.851	-36.764	1.00	24.68
BBBBATOM	2780	CA	ALA	B	27	-3.116	-40.222	-37.199	1.00	26.15
BBBBATOM	2781	CB	ALA	B	27	-3.868	-40.909	-36.066	1.00	26.23
BBBBATOM	2782	C	ALA	B	27	-3.888	-38.984	-37.661	1.00	27.60
BBBBATOM	2783	O	ALA	B	27	-4.492	-38.985	-38.736	1.00	27.05
BBBBATOM	2784	N	HIS	B	28	-3.864	-37.933	-36.847	1.00	27.68
BBBBATOM	2785	CA	HIS	B	28	-4.574	-36.702	-37.190	1.00	29.32
BBBBATOM	2786	CB	HIS	B	28	-4.498	-35.693	-36.039	1.00	27.05
BBBBATOM	2787	CG	HIS	B	28	-5.491	-35.957	-34.952	1.00	27.65
BBBBATOM	2788	CD2	HIS	B	28	-5.327	-36.213	-33.632	1.00	26.92
BBBBATOM	2789	ND1	HIS	B	28	-6.850	-36.010	-35.188	1.00	27.29
BBBBATOM	2790	CE1	HIS	B	28	-7.479	-36.290	-34.060	1.00	26.85
BBBBATOM	2791	NE2	HIS	B	28	-6.578	-36.417	-33.101	1.00	27.78
BBBBATOM	2792	C	HIS	B	28	-4.018	-36.095	-38.462	1.00	30.24
BBBBATOM	2793	O	HIS	B	28	-4.766	-35.589	-39.297	1.00	31.14
BBBBATOM	2794	N	HIS	B	29	-2.702	-36.164	-38.618	1.00	31.42
BBBBATOM	2795	CA	HIS	B	29	-2.070	-35.623	-39.806	1.00	32.38
BBBBATOM	2796	CB	HIS	B	29	-0.554	-35.764	-39.720	1.00	33.49
BBBBATOM	2797	CG	HIS	B	29	0.177	-34.957	-40.743	1.00	35.61
BBBBATOM	2798	CD2	HIS	B	29	0.667	-35.292	-41.960	1.00	36.38

BBBBATOM	2799	ND1	HIS	B	29	0.436	-33.612	-40.583	1.00	37.53
BBBBATOM	2800	CE1	HIS	B	29	1.055	-33.155	-41.657	1.00	37.93
BBBBATOM	2801	NE2	HIS	B	29	1.207	-34.154	-42.508	1.00	37.24
BBBBATOM	2802	C	HIS	B	29	-2.567	-36.324	-41.068	1.00	33.00
BBBBATOM	2803	O	HIS	B	29	-2.845	-35.674	-42.078	1.00	33.02
BBBBATOM	2804	N	LEU	B	30	-2.676	-37.650	-41.012	1.00	31.69
BBBBATOM	2805	CA	LEU	B	30	-3.136	-38.417	-42.162	1.00	32.00
BBBBATOM	2806	CB	LEU	B	30	-2.701	-39.883	-42.033	1.00	30.44
BBBBATOM	2807	CG	LEU	B	30	-1.191	-40.099	-42.203	1.00	29.95
BBBBATOM	2808	CD1	LEU	B	30	-0.823	-41.550	-41.898	1.00	28.64
BBBBATOM	2809	CD2	LEU	B	30	-0.785	-39.736	-43.621	1.00	28.97
BBBBATOM	2810	C	LEU	B	30	-4.641	-38.332	-42.375	1.00	32.37
BBBBATOM	2811	O	LEU	B	30	-5.109	-38.414	-43.507	1.00	33.16
BBBBATOM	2812	N	MET	B	31	-5.401	-38.168	-41.297	1.00	33.50
BBBBATOM	2813	CA	MET	B	31	-6.849	-38.064	-41.424	1.00	34.91
BBBBATOM	2814	CB	MET	B	31	-7.514	-38.061	-40.048	1.00	35.67
BBBBATOM	2815	CG	MET	B	31	-7.536	-39.424	-39.391	1.00	36.44
BBBBATOM	2816	SD	MET	B	31	-8.407	-39.436	-37.827	1.00	37.84
BBBBATOM	2817	CE	MET	B	31	-7.095	-39.039	-36.719	1.00	37.80
BBBBATOM	2818	C	MET	B	31	-7.197	-36.786	-42.173	1.00	35.99
BBBBATOM	2819	O	MET	B	31	-8.224	-36.710	-42.847	1.00	37.36
BBBBATOM	2820	N	ALA	B	32	-6.326	-35.791	-42.052	1.00	36.39
BBBBATOM	2821	CA	ALA	B	32	-6.510	-34.511	-42.722	1.00	37.55
BBBBATOM	2822	CB	ALA	B	32	-5.622	-33.458	-42.073	1.00	36.85
BBBBATOM	2823	C	ALA	B	32	-6.151	-34.663	-44.205	1.00	38.60
BBBBATOM	2824	O	ALA	B	32	-6.392	-33.760	-45.013	1.00	38.04
BBBBATOM	2825	N	GLN	B	33	-5.569	-35.809	-44.555	1.00	38.35
BBBBATOM	2826	CA	GLN	B	33	-5.182	-36.070	-45.938	1.00	38.24
BBBBATOM	2827	CB	GLN	B	33	-3.792	-36.706	-46.011	1.00	39.81
BBBBATOM	2828	CG	GLN	B	33	-2.771	-36.162	-45.028	1.00	41.67
BBBBATOM	2829	CD	GLN	B	33	-2.269	-34.781	-45.384	1.00	41.96
BBBBATOM	2830	OE1	GLN	B	33	-1.735	-34.559	-46.471	1.00	41.35
BBBBATOM	2831	NE2	GLN	B	33	-2.423	-33.843	-44.456	1.00	42.42
BBBBATOM	2832	C	GLN	B	33	-6.187	-37.027	-46.556	1.00	36.70
BBBBATOM	2833	O	GLN	B	33	-5.970	-37.541	-47.647	1.00	36.47
BBBBATOM	2834	N	GLY	B	34	-7.281	-37.274	-45.845	1.00	36.09
BBBBATOM	2835	CA	GLY	B	34	-8.305	-38.169	-46.353	1.00	35.75
BBBBATOM	2836	C	GLY	B	34	-8.219	-39.600	-45.837	1.00	35.33
BBBBATOM	2837	O	GLY	B	34	-9.075	-40.426	-46.146	1.00	34.43
BBBBATOM	2838	N	TRP	B	35	-7.196	-39.896	-45.042	1.00	35.23
BBBBATOM	2839	CA	TRP	B	35	-7.016	-41.246	-44.508	1.00	34.58
BBBBATOM	2840	CB	TRP	B	35	-5.618	-41.400	-43.908	1.00	35.03
BBBBATOM	2841	CG	TRP	B	35	-4.511	-41.558	-44.901	1.00	34.87
BBBBATOM	2842	CD2	TRP	B	35	-3.666	-42.704	-45.060	1.00	35.81
BBBBATOM	2843	CE2	TRP	B	35	-2.733	-42.399	-46.076	1.00	35.60
BBBBATOM	2844	CE3	TRP	B	35	-3.605	-43.961	-44.441	1.00	36.59
BBBBATOM	2845	CD1	TRP	B	35	-4.075	-40.633	-45.803	1.00	35.62
BBBBATOM	2846	NE1	TRP	B	35	-3.004	-41.129	-46.513	1.00	34.95
BBBBATOM	2847	CZ2	TRP	B	35	-1.746	-43.305	-46.488	1.00	37.19
BBBBATOM	2848	CZ3	TRP	B	35	-2.620	-44.865	-44.852	1.00	36.85
BBBBATOM	2849	CH2	TRP	B	35	-1.705	-44.528	-45.867	1.00	36.87
BBBBATOM	2850	C	TRP	B	35	-8.022	-41.670	-43.449	1.00	34.58
BBBBATOM	2851	O	TRP	B	35	-8.546	-40.850	-42.699	1.00	33.58
BBBBATOM	2852	N	GLN	B	36	-8.295	-42.969	-43.410	1.00	34.54
BBBBATOM	2853	CA	GLN	B	36	-9.175	-43.535	-42.402	1.00	35.40
BBBBATOM	2854	CB	GLN	B	36	-10.095	-44.596	-43.003	1.00	37.42
BBBBATOM	2855	CG	GLN	B	36	-11.219	-44.027	-43.862	1.00	41.66
BBBBATOM	2856	CD	GLN	B	36	-11.996	-45.103	-44.601	1.00	44.12
BBBBATOM	2857	OE1	GLN	B	36	-12.988	-44.816	-45.277	1.00	45.76
BBBBATOM	2858	NE2	GLN	B	36	-11.546	-46.350	-44.480	1.00	44.99
BBBBATOM	2859	C	GLN	B	36	-8.183	-44.186	-41.451	1.00	34.89
BBBBATOM	2860	O	GLN	B	36	-7.272	-44.885	-41.889	1.00	34.58
BBBBATOM	2861	N	VAL	B	37	-8.336	-43.941	-40.158	1.00	35.26
BBBBATOM	2862	CA	VAL	B	37	-7.417	-44.516	-39.184	1.00	34.16
BBBBATOM	2863	CB	VAL	B	37	-6.561	-43.417	-38.509	1.00	34.99
BBBBATOM	2864	CG1	VAL	B	37	-5.630	-44.032	-37.479	1.00	34.72

BBBBATOM	2865	CG2	VAL	B	37	-5.755	-42.668	-39.552	1.00	34.06
BBBBATOM	2866	C	VAL	B	37	-8.166	-45.288	-38.109	1.00	34.02
BBBBATOM	2867	O	VAL	B	37	-9.207	-44.849	-37.618	1.00	33.01
BBBBATOM	2868	N	ARG	B	38	-7.629	-46.451	-37.758	1.00	32.20
BBBBATOM	2869	CA	ARG	B	38	-8.219	-47.286	-36.730	1.00	31.56
BBBBATOM	2870	CB	ARG	B	38	-8.811	-48.554	-37.344	1.00	33.53
BBBBATOM	2871	CG	ARG	B	38	-9.706	-49.324	-36.397	1.00	36.77
BBBBATOM	2872	CD	ARG	B	38	-11.107	-49.511	-36.975	1.00	38.80
BBBBATOM	2873	NE	ARG	B	38	-12.000	-50.108	-35.989	1.00	41.24
BBBBATOM	2874	CZ	ARG	B	38	-13.304	-50.293	-36.161	1.00	43.18
BBBBATOM	2875	NH1	ARG	B	38	-13.892	-49.927	-37.294	1.00	43.21
BBBBATOM	2876	NH2	ARG	B	38	-14.026	-50.839	-35.189	1.00	44.37
BBBBATOM	2877	C	ARG	B	38	-7.097	-47.628	-35.751	1.00	30.48
BBBBATOM	2878	O	ARG	B	38	-5.936	-47.742	-36.134	1.00	29.62
BBBBATOM	2879	N	TRP	B	39	-7.447	-47.782	-34.484	1.00	28.40
BBBBATOM	2880	CA	TRP	B	39	-6.456	-48.070	-33.471	1.00	27.41
BBBBATOM	2881	CB	TRP	B	39	-6.696	-47.145	-32.291	1.00	27.98
BBBBATOM	2882	CG	TRP	B	39	-5.480	-46.788	-31.568	1.00	28.00
BBBBATOM	2883	CD2	TRP	B	39	-4.677	-45.627	-31.784	1.00	28.42
BBBBATOM	2884	CE2	TRP	B	39	-3.625	-45.673	-30.851	1.00	28.85
BBBBATOM	2885	CE3	TRP	B	39	-4.749	-44.549	-32.680	1.00	29.78
BBBBATOM	2886	CD1	TRP	B	39	-4.898	-47.476	-30.549	1.00	28.26
BBBBATOM	2887	NE1	TRP	B	39	-3.783	-46.812	-30.111	1.00	28.48
BBBBATOM	2888	CZ2	TRP	B	39	-2.648	-44.684	-30.778	1.00	30.55
BBBBATOM	2889	CZ3	TRP	B	39	-3.770	-43.561	-32.610	1.00	29.22
BBBBATOM	2890	CH2	TRP	B	39	-2.734	-43.639	-31.662	1.00	30.90
BBBBATOM	2891	C	TRP	B	39	-6.478	-49.517	-32.999	1.00	25.82
BBBBATOM	2892	O	TRP	B	39	-7.509	-50.176	-33.055	1.00	24.87
BBBBATOM	2893	N	LEU	B	40	-5.323	-50.004	-32.549	1.00	25.21
BBBBATOM	2894	CA	LEU	B	40	-5.200	-51.364	-32.026	1.00	24.71
BBBBATOM	2895	CB	LEU	B	40	-4.326	-52.221	-32.952	1.00	25.21
BBBBATOM	2896	CG	LEU	B	40	-4.416	-53.754	-32.868	1.00	26.95
BBBBATOM	2897	CD1	LEU	B	40	-3.037	-54.334	-32.571	1.00	27.63
BBBBATOM	2898	CD2	LEU	B	40	-5.421	-54.179	-31.817	1.00	26.69
BBBBATOM	2899	C	LEU	B	40	-4.535	-51.235	-30.655	1.00	23.33
BBBBATOM	2900	O	LEU	B	40	-3.387	-50.824	-30.563	1.00	23.43
BBBBATOM	2901	N	GLY	B	41	-5.260	-51.567	-29.591	1.00	24.01
BBBBATOM	2902	CA	GLY	B	41	-4.691	-51.450	-28.257	1.00	23.47
BBBBATOM	2903	C	GLY	B	41	-5.292	-52.479	-27.322	1.00	23.99
BBBBATOM	2904	O	GLY	B	41	-5.797	-53.498	-27.785	1.00	22.90
BBBBATOM	2905	N	THR	B	42	-5.225	-52.225	-26.017	1.00	26.62
BBBBATOM	2906	CA	THR	B	42	-5.787	-53.141	-25.027	1.00	29.84
BBBBATOM	2907	CB	THR	B	42	-4.693	-53.715	-24.092	1.00	30.17
BBBBATOM	2908	OG1	THR	B	42	-4.019	-52.647	-23.418	1.00	30.77
BBBBATOM	2909	CG2	THR	B	42	-3.683	-54.514	-24.900	1.00	31.30
BBBBATOM	2910	C	THR	B	42	-6.852	-52.420	-24.200	1.00	32.04
BBBBATOM	2911	O	THR	B	42	-6.737	-51.226	-23.924	1.00	31.27
BBBBATOM	2912	N	ALA	B	43	-7.881	-53.160	-23.801	1.00	35.37
BBBBATOM	2913	CA	ALA	B	43	-9.000	-52.595	-23.047	1.00	38.81
BBBBATOM	2914	CB	ALA	B	43	-10.063	-53.669	-22.835	1.00	38.49
BBBBATOM	2915	C	ALA	B	43	-8.671	-51.928	-21.713	1.00	41.06
BBBBATOM	2916	O	ALA	B	43	-9.224	-50.875	-21.391	1.00	42.22
BBBBATOM	2917	N	ASP	B	44	-7.777	-52.521	-20.931	1.00	43.18
BBBBATOM	2918	CA	ASP	B	44	-7.455	-51.942	-19.632	1.00	44.47
BBBBATOM	2919	CB	ASP	B	44	-7.311	-53.057	-18.586	1.00	46.93
BBBBATOM	2920	CG	ASP	B	44	-8.646	-53.724	-18.255	1.00	48.65
BBBBATOM	2921	OD1	ASP	B	44	-9.553	-53.026	-17.753	1.00	50.52
BBBBATOM	2922	OD2	ASP	B	44	-8.791	-54.943	-18.498	1.00	49.40
BBBBATOM	2923	C	ASP	B	44	-6.236	-51.025	-19.598	1.00	44.13
BBBBATOM	2924	O	ASP	B	44	-5.520	-50.968	-18.595	1.00	45.05
BBBBATOM	2925	N	ARG	B	45	-6.001	-50.307	-20.692	1.00	42.34
BBBBATOM	2926	CA	ARG	B	45	-4.887	-49.367	-20.763	1.00	40.44
BBBBATOM	2927	CB	ARG	B	45	-3.802	-49.869	-21.725	1.00	41.87
BBBBATOM	2928	CG	ARG	B	45	-2.935	-50.994	-21.149	1.00	43.86
BBBBATOM	2929	CD	ARG	B	45	-2.218	-50.541	-19.881	1.00	45.24
BBBBATOM	2930	NE	ARG	B	45	-1.385	-51.582	-19.277	1.00	46.96

BBBBATOM	2931	CZ	ARG	B	45	-1.840	-52.753	-18.839	1.00	47.69
BBBBATOM	2932	NH1	ARG	B	45	-3.130	-53.961	-18.937	1.00	48.59
BBBBATOM	2933	NH2	ARG	B	45	-1.005	-53.626	-18.289	1.00	48.33
BBBBATOM	2934	C	ARG	B	45	-5.390	-47.992	-21.195	1.00	38.74
BBBBATOM	2935	O	ARG	B	45	-6.486	-47.866	-21.738	1.00	37.69
BBBBATOM	2936	N	MET	B	46	-4.567	-46.977	-20.955	1.00	37.09
BBBBATOM	2937	CA	MET	B	46	-4.881	-45.581	-21.249	1.00	36.33
BBBBATOM	2938	CB	MET	B	46	-3.644	-44.725	-20.945	1.00	37.92
BBBBATOM	2939	CG	MET	B	46	-3.873	-43.222	-20.952	1.00	40.65
BBBBATOM	2940	SD	MET	B	46	-3.420	-42.436	-22.517	1.00	44.22
BBBBATOM	2941	CE	MET	B	46	-1.720	-41.959	-22.168	1.00	41.80
BBBBATOM	2942	C	MET	B	46	-5.430	-45.239	-22.643	1.00	34.96
BBBBATOM	2943	O	MET	B	46	-6.264	-44.338	-22.774	1.00	33.21
BBBBATOM	2944	N	GLU	B	47	-4.976	-45.941	-23.678	1.00	32.85
BBBBATOM	2945	CA	GLU	B	47	-5.458	-45.655	-25.029	1.00	31.79
BBBBATOM	2946	CB	GLU	B	47	-4.624	-46.402	-26.080	1.00	30.62
BBBBATOM	2947	CG	GLU	B	47	-4.755	-47.922	-26.051	1.00	29.85
BBBBATOM	2948	CD	GLU	B	47	-3.793	-48.597	-25.082	1.00	29.78
BBBBATOM	2949	OE1	GLU	B	47	-3.188	-47.895	-24.247	1.00	28.76
BBBBATOM	2950	OE2	GLU	B	47	-3.649	-49.840	-25.156	1.00	29.01
BBBBATOM	2951	C	GLU	B	47	-6.938	-46.017	-25.191	1.00	31.81
BBBBATOM	2952	O	GLU	B	47	-7.626	-45.476	-26.055	1.00	31.31
BBBBATOM	2953	N	ALA	B	48	-7.428	-46.924	-24.352	1.00	31.55
BBBBATOM	2954	CA	ALA	B	48	-8.821	-47.344	-24.414	1.00	32.58
BBBBATOM	2955	CB	ALA	B	48	-9.085	-48.450	-23.384	1.00	33.19
BBBBATOM	2956	C	ALA	B	48	-9.761	-46.168	-24.164	1.00	33.37
BBBBATOM	2957	O	ALA	B	48	-10.860	-46.114	-24.716	1.00	33.81
BBBBATOM	2958	N	ASP	B	49	-9.328	-45.232	-23.328	1.00	34.05
BBBBATOM	2959	CA	ASP	B	49	-10.143	-44.065	-23.009	1.00	35.60
BBBBATOM	2960	CB	ASP	B	49	-10.033	-43.736	-21.514	1.00	36.58
BBBBATOM	2961	CG	ASP	B	49	-10.645	-44.812	-20.628	1.00	39.54
BBBBATOM	2962	OD1	ASP	B	49	-11.835	-45.144	-20.825	1.00	40.82
BBBBATOM	2963	OD2	ASP	B	49	-9.939	-45.323	-19.730	1.00	39.49
BBBBATOM	2964	C	ASP	B	49	-9.768	-42.832	-23.831	1.00	34.79
BBBBATOM	2965	O	ASP	B	49	-10.637	-42.064	-24.241	1.00	35.85
BBBBATOM	2966	N	LEU	B	50	-8.478	-42.648	-24.088	1.00	34.06
BBBBATOM	2967	CA	LEU	B	50	-8.026	-41.484	-24.840	1.00	33.49
BBBBATOM	2968	CB	LEU	B	50	-6.526	-41.264	-24.635	1.00	33.25
BBBBATOM	2969	CG	LEU	B	50	-6.001	-39.986	-25.299	1.00	33.36
BBBBATOM	2970	CD1	LEU	B	50	-6.679	-38.771	-24.659	1.00	34.04
BBBBATOM	2971	CD2	LEU	B	50	-4.496	-39.894	-25.157	1.00	33.08
BBBBATOM	2972	C	LEU	B	50	-8.320	-41.486	-26.337	1.00	33.52
BBBBATOM	2973	O	LEU	B	50	-8.769	-40.477	-26.882	1.00	32.52
BBBBATOM	2974	N	VAL	B	51	-8.073	-42.605	-27.011	1.00	32.94
BBBBATOM	2975	CA	VAL	B	51	-8.299	-42.641	-28.449	1.00	32.68
BBBBATOM	2976	CB	VAL	B	51	-7.829	-43.982	-29.058	1.00	33.06
BBBBATOM	2977	CG1	VAL	B	51	-8.115	-44.013	-30.565	1.00	31.54
BBBBATOM	2978	CG2	VAL	B	51	-6.329	-44.145	-28.813	1.00	31.45
BBBBATOM	2979	C	VAL	B	51	-9.747	-42.348	-28.829	1.00	33.08
BBBBATOM	2980	O	VAL	B	51	-10.000	-41.623	-29.792	1.00	32.88
BBBBATOM	2981	N	PRO	B	52	-10.721	-42.900	-28.085	1.00	33.67
BBBBATOM	2982	CD	PRO	B	52	-10.667	-44.012	-27.119	1.00	33.29
BBBBATOM	2983	CA	PRO	B	52	-12.111	-42.601	-28.453	1.00	34.43
BBBBATOM	2984	CB	PRO	B	52	-12.915	-43.465	-27.489	1.00	34.36
BBBBATOM	2985	CG	PRO	B	52	-12.021	-44.661	-27.307	1.00	33.77
BBBBATOM	2986	C	PRO	B	52	-12.422	-41.111	-28.294	1.00	35.67
BBBBATOM	2987	O	PRO	B	52	-13.219	-40.548	-29.048	1.00	36.65
BBBBATOM	2988	N	LYS	B	53	-11.790	-40.478	-27.310	1.00	35.75
BBBBATOM	2989	CA	LYS	B	53	-11.998	-39.054	-27.064	1.00	36.73
BBBBATOM	2990	CB	LYS	B	53	-11.334	-38.633	-25.746	1.00	37.14
BBBBATOM	2991	CG	LYS	B	53	-12.020	-39.207	-24.514	1.00	38.38
BBBBATOM	2992	CD	LYS	B	53	-11.368	-38.746	-23.218	1.00	39.34
BBBBATOM	2993	CE	LYS	B	53	-12.057	-39.379	-22.012	1.00	40.74
BBBBATOM	2994	NZ	LYS	B	53	-11.352	-39.092	-20.725	1.00	40.94
BBBBATOM	2995	C	LYS	B	53	-11.445	-38.231	-28.220	1.00	36.11
BBBBATOM	2996	O	LYS	B	53	-11.703	-37.036	-28.323	1.00	36.71

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BBBBATOM   2997  N   HIS B  54     -10.688 -38.881 -29.096  1.00 35.60
BBBBATOM   2998  CA  HIS B  54     -10.116 -38.212 -30.259  1.00 34.62
BBBBATOM   2999  CB  HIS B  54      -8.666 -38.647 -30.464  1.00 34.78
BBBBATOM   3000  CG  HIS B  54      -7.676 -37.810 -29.721  1.00 33.79
BBBBATOM   3001  CD2 HIS B  54      -7.360 -37.760 -28.406  1.00 33.76
BBBBATOM   3002  ND1 HIS B  54      -6.884 -36.869 -30.343  1.00 34.27
BBBBATOM   3003  CE1 HIS B  54      -6.120 -36.277 -29.441  1.00 34.41
BBBBATOM   3004  NE2 HIS B  54      -6.390 -36.799 -28.258  1.00 33.91
BBBBATOM   3005  C   HIS B  54     -10.919 -38.524 -31.512  1.00 34.28
BBBBATOM   3006  O   HIS B  54     -10.487 -38.224 -32.620  1.00 34.99
BBBBATOM   3007  N   GLY B  55     -12.082 -39.140 -31.325  1.00 34.47
BBBBATOM   3008  CA  GLY B  55     -12.938 -39.481 -32.447  1.00 35.34
BBBBATOM   3009  C   GLY B  55     -12.427 -40.619 -33.310  1.00 36.18
BBBBATOM   3010  O   GLY B  55     -12.883 -40.799 -34.442  1.00 35.99
BBBBATOM   3011  N   ILE B  56     -11.490 -41.399 -32.776  1.00 35.32
BBBBATOM   3012  CA  ILE B  56     -10.909 -42.517 -33.514  1.00 33.81
BBBBATOM   3013  CB  ILE B  56      -9.374 -42.445 -33.462  1.00 33.36
BBBBATOM   3014  CG2 ILE B  56      -8.761 -43.602 -34.245  1.00 32.87
BBBBATOM   3015  CG1 ILE B  56      -8.916 -41.097 -34.029  1.00 32.05
BBBBATOM   3016  CD1 ILE B  56      -7.461 -40.792 -33.818  1.00 30.35
BBBBATOM   3017  C   ILE B  56     -11.375 -43.859 -32.956  1.00 34.45
BBBBATOM   3018  O   ILE B  56     -11.394 -44.069 -31.738  1.00 34.26
BBBBATOM   3019  N   GLU B  57     -11.764 -44.758 -33.855  1.00 33.40
BBBBATOM   3020  CA  GLU B  57     -12.228 -46.083 -33.467  1.00 34.16
BBBBATOM   3021  CB  GLU B  57     -12.905 -46.769 -34.651  1.00 37.41
BBBBATOM   3022  CG  GLU B  57     -14.064 -45.982 -35.244  1.00 42.10
BBBBATOM   3023  CD  GLU B  57     -14.653 -46.659 -36.465  1.00 45.50
BBBBATOM   3024  OE1 GLU B  57     -13.903 -46.875 -37.448  1.00 46.39
BBBBATOM   3025  OE2 GLU B  57     -15.866 -46.977 -36.441  1.00 48.36
BBBBATOM   3026  C   GLU B  57     -11.044 -46.923 -33.005  1.00 33.01
BBBBATOM   3027  O   GLU B  57      -9.931 -46.769 -33.504  1.00 31.58
BBBBATOM   3028  N   ILE B  58     -11.287 -47.817 -32.056  1.00 31.85
BBBBATOM   3029  CA  ILE B  58     -10.217 -48.658 -31.553  1.00 31.38
BBBBATOM   3030  CB  ILE B  58      -9.651 -48.099 -30.223  1.00 30.95
BBBBATOM   3031  CG2 ILE B  58     -10.769 -47.946 -29.205  1.00 31.48
BBBBATOM   3032  CG1 ILE B  58      -8.553 -49.030 -29.690  1.00 31.13
BBBBATOM   3033  CD1 ILE B  58      -7.736 -48.437 -28.572  1.00 29.87
BBBBATOM   3034  C   ILE B  58     -10.647 -50.102 -31.357  1.00 31.67
BBBBATOM   3035  O   ILE B  58     -11.716 -50.384 -30.801  1.00 30.68
BBBBATOM   3036  N   ASP B  59      -9.807 -51.011 -31.844  1.00 30.76
BBBBATOM   3037  CA  ASP B  59     -10.039 -52.442 -31.720  1.00 31.09
BBBBATOM   3038  CB  ASP B  59      -9.732 -53.153 -33.037  1.00 31.37
BBBBATOM   3039  CG  ASP B  59     -10.766 -52.863 -34.104  1.00 32.68
BBBBATOM   3040  OD1 ASP B  59     -11.969 -53.037 -33.812  1.00 32.40
BBBBATOM   3041  OD2 ASP B  59     -10.378 -52.468 -35.224  1.00 33.40
BBBBATOM   3042  C   ASP B  59      -9.119 -52.950 -30.618  1.00 30.50
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BBBBATOM   3044  N   PHE B  60      -9.608 -53.888 -29.815  1.00 30.65
BBBBATOM   3045  CA  PHE B  60      -8.809 -54.410 -28.713  1.00 30.32
BBBBATOM   3046  CB  PHE B  60      -9.560 -54.239 -27.385  1.00 30.74
BBBBATOM   3047  CG  PHE B  60      -9.925 -52.815 -27.058  1.00 32.14
BBBBATOM   3048  CD1 PHE B  60     -11.250 -52.392 -27.129  1.00 33.15
BBBBATOM   3049  CD2 PHE B  60      -8.955 -51.908 -26.649  1.00 31.57
BBBBATOM   3050  CE1 PHE B  60     -11.605 -51.083 -26.791  1.00 34.05
BBBBATOM   3051  CE2 PHE B  60      -9.294 -50.598 -26.310  1.00 33.00
BBBBATOM   3052  CZ  PHE B  60     -10.626 -50.185 -26.380  1.00 33.82
BBBBATOM   3053  C   PHE B  60      -8.430 -55.878 -28.846  1.00 29.86
BBBBATOM   3054  O   PHE B  60      -9.154 -56.668 -29.445  1.00 29.93
BBBBATOM   3055  N   ILE B  61      -7.271 -56.229 -28.295  1.00 29.38
BBBBATOM   3056  CA  ILE B  61      -6.832 -57.616 -28.269  1.00 28.55
BBBBATOM   3057  CB  ILE B  61      -5.674 -57.923 -29.258  1.00 28.48
BBBBATOM   3058  CG2 ILE B  61      -6.123 -57.650 -30.694  1.00 27.65
BBBBATOM   3059  CG1 ILE B  61      -4.422 -57.126 -28.892  1.00 26.70
BBBBATOM   3060  CD1 ILE B  61      -3.177 -57.615 -29.638  1.00 27.03
BBBBATOM   3061  C   ILE B  61      -6.344 -57.855 -26.848  1.00 29.13
BBBBATOM   3062  O   ILE B  61      -6.124 -56.906 -26.091  1.00 28.80
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BBBBATOM	3063	N	ARG	B	62	-6.186	-59.116	-26.473	1.00	29.38
BBBBATOM	3064	CA	ARG	B	62	-5.709	-59.416	-25.133	1.00	30.76
BBBBATOM	3065	CB	ARG	B	62	-6.630	-60.447	-24.461	1.00	32.36
BBBBATOM	3066	CG	ARG	B	62	-6.130	-60.955	-23.114	1.00	35.99
BBBBATOM	3067	CD	ARG	B	62	-5.438	-59.859	-22.311	1.00	37.86
BBBBATOM	3068	NE	ARG	B	62	-6.297	-58.718	-22.004	1.00	40.01
BBBBATOM	3069	CZ	ARG	B	62	-5.840	-57.504	-21.711	1.00	39.09
BBBBATOM	3070	NH1	ARG	B	62	-4.536	-57.275	-21.690	1.00	39.24
BBBBATOM	3071	NH2	ARG	B	62	-6.686	-56.518	-21.439	1.00	40.03
BBBBATOM	3072	C	ARG	B	62	-4.274	-59.923	-25.156	1.00	29.32
BBBBATOM	3073	O	ARG	B	62	-3.933	-60.809	-25.934	1.00	28.65
BBBBATOM	3074	N	ILE	B	63	-3.428	-59.342	-24.313	1.00	30.07
BBBBATOM	3075	CA	ILE	B	63	-2.036	-59.770	-24.231	1.00	31.38
BBBBATOM	3076	CB	ILE	B	63	-1.081	-58.745	-24.883	1.00	30.06
BBBBATOM	3077	CG2	ILE	B	63	-1.442	-58.567	-26.353	1.00	30.41
BBBBATOM	3078	CG1	ILE	B	63	-1.143	-57.411	-24.137	1.00	29.94
BBBBATOM	3079	CD1	ILE	B	63	-0.128	-56.384	-24.632	1.00	29.62
BBBBATOM	3080	C	ILE	B	63	-1.623	-59.981	-22.775	1.00	33.08
BBBBATOM	3081	O	ILE	B	63	-0.444	-59.872	-22.430	1.00	33.21
BBBBATOM	3082	N	SER	B	64	-2.603	-60.284	-21.927	1.00	35.38
BBBBATOM	3083	CA	SER	B	64	-2.356	-60.520	-20.505	1.00	37.51
BBBBATOM	3084	CB	SER	B	64	-3.652	-60.912	-19.792	1.00	38.82
BBBBATOM	3085	OG	SER	B	64	-4.558	-59.823	-19.750	1.00	42.88
BBBBATOM	3086	C	SER	B	64	-1.326	-61.622	-20.311	1.00	37.32
BBBBATOM	3087	O	SER	B	64	-1.411	-62.682	-20.933	1.00	37.86
BBBBATOM	3088	N	GLY	B	65	-0.356	-61.370	-19.441	1.00	37.81
BBBBATOM	3089	CA	GLY	B	65	0.679	-62.355	-19.199	1.00	37.13
BBBBATOM	3090	C	GLY	B	65	1.798	-62.283	-20.226	1.00	36.76
BBBBATOM	3091	O	GLY	B	65	2.858	-62.889	-20.038	1.00	37.57
BBBBATOM	3092	N	LEU	B	66	1.577	-61.539	-21.307	1.00	34.63
BBBBATOM	3093	CA	LEU	B	66	2.591	-61.413	-22.355	1.00	33.17
BBBBATOM	3094	CB	LEU	B	66	1.936	-61.470	-23.735	1.00	32.08
BBBBATOM	3095	CG	LEU	B	66	1.162	-62.747	-24.061	1.00	32.52
BBBBATOM	3096	CD1	LEU	B	66	0.563	-62.626	-25.445	1.00	31.38
BBBBATOM	3097	CD2	LEU	B	66	2.093	-63.957	-23.984	1.00	31.67
BBBBATOM	3098	C	LEU	B	66	3.414	-60.133	-22.246	1.00	32.72
BBBBATOM	3099	O	LEU	B	66	4.451	-60.002	-22.893	1.00	33.13
BBBBATOM	3100	N	ARG	B	67	2.953	-59.185	-21.440	1.00	31.54
BBBBATOM	3101	CA	ARG	B	67	3.671	-57.928	-21.277	1.00	30.90
BBBBATOM	3102	CB	ARG	B	67	2.888	-56.984	-20.363	1.00	32.28
BBBBATOM	3103	CG	ARG	B	67	1.540	-56.576	-20.913	1.00	34.65
BBBBATOM	3104	CD	ARG	B	67	0.926	-55.440	-20.097	1.00	36.69
BBBBATOM	3105	NE	ARG	B	67	-0.259	-54.889	-20.748	1.00	38.28
BBBBATOM	3106	CZ	ARG	B	67	-1.425	-55.519	-20.853	1.00	39.05
BBBBATOM	3107	NH1	ARG	B	67	-1.583	-56.734	-20.341	1.00	39.61
BBBBATOM	3108	NH2	ARG	B	67	-2.434	-54.935	-21.487	1.00	39.52
BBBBATOM	3109	C	ARG	B	67	5.071	-58.142	-20.713	1.00	29.99
BBBBATOM	3110	O	ARG	B	67	5.294	-59.034	-19.889	1.00	28.67
BBBBATOM	3111	N	GLY	B	68	6.014	-57.321	-21.165	1.00	27.75
BBBBATOM	3112	CA	GLY	B	68	7.380	-57.427	-20.685	1.00	26.79
BBBBATOM	3113	C	GLY	B	68	8.166	-58.579	-21.280	1.00	25.41
BBBBATOM	3114	O	GLY	B	68	9.326	-58.779	-20.943	1.00	26.04
BBBBATOM	3115	N	LYS	B	69	7.546	-59.342	-22.170	1.00	24.55
BBBBATOM	3116	CA	LYS	B	69	8.238	-60.463	-22.796	1.00	23.93
BBBBATOM	3117	CB	LYS	B	69	7.284	-61.641	-23.033	1.00	24.12
BBBBATOM	3118	CG	LYS	B	69	6.757	-62.360	-21.794	1.00	25.08
BBBBATOM	3119	CD	LYS	B	69	5.887	-63.553	-22.224	1.00	25.44
BBBBATOM	3120	CE	LYS	B	69	5.357	-64.358	-21.035	1.00	28.31
BBBBATOM	3121	NZ	LYS	B	69	6.468	-64.877	-20.175	1.00	29.71
BBBBATOM	3122	C	LYS	B	69	8.825	-60.062	-24.142	1.00	23.32
BBBBATOM	3123	O	LYS	B	69	8.151	-59.404	-24.944	1.00	21.96
BBBBATOM	3124	N	GLY	B	70	10.075	-60.470	-24.374	1.00	22.48
BBBBATOM	3125	CA	GLY	B	70	10.755	-60.229	-25.636	1.00	22.26
BBBBATOM	3126	C	GLY	B	70	10.308	-61.337	-26.588	1.00	22.17
BBBBATOM	3127	O	GLY	B	70	9.512	-62.183	-26.195	1.00	21.62
BBBBATOM	3128	N	ILE	B	71	10.819	-61.373	-27.814	1.00	21.85

BBBBATOM	3129	CA	ILE	B	71	10.357	-62.386	-28.762	1.00 23.55
BBBBATOM	3130	CB	ILE	B	71	10.926	-62.142	-30.181	1.00 23.52
BBBBATOM	3131	CG2	ILE	B	71	12.435	-62.375	-30.192	1.00 25.96
BBBBATOM	3132	CG1	ILE	B	71	10.264	-63.096	-31.182	1.00 24.18
BBBBATOM	3133	CD1	ILE	B	71	8.745	-62.981	-31.263	1.00 25.73
BBBBATOM	3134	C	ILE	B	71	10.616	-63.840	-28.359	1.00 23.88
BBBBATOM	3135	O	ILE	B	71	9.775	-64.707	-28.592	1.00 21.66
BBBBATOM	3136	N	LYS	B	72	11.764	-64.119	-27.751	1.00 23.82
BBBBATOM	3137	CA	LYS	B	72	12.038	-65.491	-27.343	1.00 24.92
BBBBATOM	3138	CB	LYS	B	72	13.491	-65.634	-26.875	1.00 26.86
BBBBATOM	3139	CG	LYS	B	72	14.496	-65.590	-28.019	1.00 31.29
BBBBATOM	3140	CD	LYS	B	72	15.925	-65.791	-27.518	1.00 36.00
BBBBATOM	3141	CE	LYS	B	72	16.926	-65.816	-28.671	1.00 38.82
BBBBATOM	3142	NZ	LYS	B	72	18.342	-65.957	-28.192	1.00 41.21
BBBBATOM	3143	C	LYS	B	72	11.068	-65.925	-26.245	1.00 23.73
BBBBATOM	3144	O	LYS	B	72	10.592	-67.062	-26.245	1.00 24.08
BBBBATOM	3145	N	ALA	B	73	10.765	-65.016	-25.322	1.00 21.62
BBBBATOM	3146	CA	ALA	B	73	9.839	-65.306	-24.233	1.00 21.18
BBBBATOM	3147	CB	ALA	B	73	9.895	-64.196	-23.187	1.00 22.25
BBBBATOM	3148	C	ALA	B	73	8.412	-65.454	-24.771	1.00 20.36
BBBBATOM	3149	O	ALA	B	73	7.619	-66.250	-24.267	1.00 18.97
BBBBATOM	3150	N	LEU	B	74	8.076	-64.673	-25.791	1.00 20.23
BBBBATOM	3151	CA	LEU	B	74	6.745	-64.762	-26.387	1.00 19.36
BBBBATOM	3152	CB	LEU	B	74	6.540	-63.643	-27.417	1.00 18.42
BBBBATOM	3153	CG	LEU	B	74	6.422	-62.208	-26.884	1.00 18.80
BBBBATOM	3154	CD1	LEU	B	74	6.473	-61.197	-28.039	1.00 19.86
BBBBATOM	3155	CD2	LEU	B	74	5.109	-62.071	-26.104	1.00 19.45
BBBBATOM	3156	C	LEU	B	74	6.549	-66.110	-27.069	1.00 19.37
BBBBATOM	3157	O	LEU	B	74	5.539	-66.779	-26.863	1.00 20.01
BBBBATOM	3158	N	ILE	B	75	7.520	-66.507	-27.883	1.00 20.59
BBBBATOM	3159	CA	ILE	B	75	7.434	-67.768	-28.601	1.00 21.18
BBBBATOM	3160	CB	ILE	B	75	8.571	-67.896	-29.641	1.00 22.95
BBBBATOM	3161	CG2	ILE	B	75	8.334	-69.108	-30.527	1.00 25.38
BBBBATOM	3162	CG1	ILE	B	75	8.598	-66.657	-30.540	1.00 26.82
BBBBATOM	3163	CD1	ILE	B	75	7.304	-66.442	-31.327	1.00 28.48
BBBBATOM	3164	C	ILE	B	75	7.488	-68.942	-27.624	1.00 21.20
BBBBATOM	3165	O	ILE	B	75	7.125	-70.063	-27.979	1.00 21.59
BBBBATOM	3166	N	ALA	B	76	7.940	-68.680	-26.399	1.00 20.49
BBBBATOM	3167	CA	ALA	B	76	7.996	-69.726	-25.374	1.00 21.72
BBBBATOM	3168	CB	ALA	B	76	9.026	-69.372	-24.305	1.00 21.92
BBBBATOM	3169	C	ALA	B	76	6.624	-69.904	-24.732	1.00 21.54
BBBBATOM	3170	O	ALA	B	76	6.441	-70.778	-23.875	1.00 20.75
BBBBATOM	3171	N	ALA	B	77	5.668	-69.066	-25.145	1.00 20.61
BBBBATOM	3172	CA	ALA	B	77	4.289	-69.121	-24.655	1.00 21.07
BBBBATOM	3173	CB	ALA	B	77	3.937	-67.830	-23.924	1.00 20.10
BBBBATOM	3174	C	ALA	B	77	3.383	-69.298	-25.881	1.00 21.69
BBBBATOM	3175	O	ALA	B	77	2.567	-68.430	-26.199	1.00 21.93
BBBBATOM	3176	N	PRO	B	78	3.507	-70.446	-26.564	1.00 22.38
BBBBATOM	3177	CD	PRO	B	78	4.211	-71.603	-25.976	1.00 21.89
BBBBATOM	3178	CA	PRO	B	78	2.772	-70.846	-27.771	1.00 20.95
BBBBATOM	3179	CB	PRO	B	78	3.027	-72.350	-27.861	1.00 22.21
BBBBATOM	3180	CG	PRO	B	78	4.288	-72.547	-27.117	1.00 24.07
BBBBATOM	3181	C	PRO	B	78	1.278	-70.535	-27.813	1.00 21.19
BBBBATOM	3182	O	PRO	B	78	0.789	-69.939	-28.776	1.00 19.68
BBBBATOM	3183	N	LEU	B	79	0.544	-70.961	-26.790	1.00 21.21
BBBBATOM	3184	CA	LEU	B	79	-0.896	-70.728	-26.783	1.00 21.32
BBBBATOM	3185	CB	LEU	B	79	-1.569	-71.476	-25.630	1.00 20.99
BBBBATOM	3186	CG	LEU	B	79	-1.397	-72.988	-25.617	1.00 22.40
BBBBATOM	3187	CD1	LEU	B	79	-2.504	-73.619	-24.772	1.00 22.01
BBBBATOM	3188	CD2	LEU	B	79	-1.438	-73.521	-27.021	1.00 23.82
BBBBATOM	3189	C	LEU	B	79	-1.275	-69.263	-26.707	1.00 21.17
BBBBATOM	3190	O	LEU	B	79	-2.125	-68.800	-27.481	1.00 20.44
BBBBATOM	3191	N	ARG	B	80	-0.656	-68.529	-25.788	1.00 20.91
BBBBATOM	3192	CA	ARG	B	80	-0.980	-67.115	-25.637	1.00 21.30
BBBBATOM	3193	CB	ARG	B	80	-0.444	-66.583	-24.312	1.00 22.12
BBBBATOM	3194	CG	ARG	B	80	-1.286	-67.051	-23.118	1.00 24.03

BBBBATOM	3195	CD	ARG	B	80	-0.610	-66.738	-21.807	1.00	23.42
BBBBATOM	3196	NE	ARG	B	80	0.581	-67.556	-21.610	1.00	24.59
BBBBATOM	3197	CZ	ARG	B	80	1.466	-67.351	-20.642	1.00	26.08
BBBBATOM	3198	NH1	ARG	B	80	1.290	-66.349	-19.787	1.00	26.92
BBBBATOM	3199	NH2	ARG	B	80	2.514	-68.152	-20.519	1.00	27.22
BBBBATOM	3200	C	ARG	B	80	-0.526	-66.233	-26.790	1.00	21.29
BBBBATOM	3201	O	ARG	B	80	-1.278	-65.355	-27.223	1.00	21.47
BBBBATOM	3202	N	ILE	B	81	0.683	-66.448	-27.303	1.00	19.29
BBBBATOM	3203	CA	ILE	B	81	1.113	-65.621	-28.421	1.00	19.47
BBBBATOM	3204	CB	ILE	B	81	2.639	-65.793	-28.730	1.00	17.92
BBBBATOM	3205	CG2	ILE	B	81	2.949	-67.200	-29.206	1.00	17.33
BBBBATOM	3206	CG1	ILE	B	81	3.067	-64.753	-29.769	1.00	18.63
BBBBATOM	3207	CD1	ILE	B	81	2.746	-63.318	-29.346	1.00	17.46
BBBBATOM	3208	C	ILE	B	81	0.256	-65.937	-29.654	1.00	18.99
BBBBATOM	3209	O	ILE	B	81	-0.149	-65.028	-30.378	1.00	19.38
BBBBATOM	3210	N	PHE	B	82	-0.056	-67.211	-29.880	1.00	19.39
BBBBATOM	3211	CA	PHE	B	82	-0.875	-67.582	-31.038	1.00	19.15
BBBBATOM	3212	CB	PHE	B	82	-1.057	-69.103	-31.136	1.00	19.27
BBBBATOM	3213	CG	PHE	B	82	-1.811	-69.548	-32.368	1.00	19.87
BBBBATOM	3214	CD1	PHE	B	82	-1.180	-69.602	-33.603	1.00	20.87
BBBBATOM	3215	CD2	PHE	B	82	-3.154	-69.898	-32.289	1.00	21.11
BBBBATOM	3216	CE1	PHE	B	82	-1.872	-70.002	-34.753	1.00	21.20
BBBBATOM	3217	CE2	PHE	B	82	-3.857	-70.297	-33.429	1.00	22.26
BBBBATOM	3218	CZ	PHE	B	82	-3.212	-70.349	-34.663	1.00	22.14
BBBBATOM	3219	C	PHE	B	82	-2.250	-66.931	-30.959	1.00	19.94
BBBBATOM	3220	O	PHE	B	82	-2.777	-66.444	-31.970	1.00	19.64
BBBBATOM	3221	N	ASN	B	83	-2.832	-66.923	-29.764	1.00	19.29
BBBBATOM	3222	CA	ASN	B	83	-4.150	-66.332	-29.577	1.00	20.90
BBBBATOM	3223	CB	ASN	B	83	-4.693	-66.641	-28.178	1.00	20.55
BBBBATOM	3224	CG	ASN	B	83	-6.158	-66.244	-28.028	1.00	22.79
BBBBATOM	3225	OD1	ASN	B	83	-6.505	-65.374	-27.229	1.00	25.14
BBBBATOM	3226	ND2	ASN	B	83	-7.018	-66.877	-28.807	1.00	20.47
BBBBATOM	3227	C	ASN	B	83	-4.178	-64.821	-29.812	1.00	20.83
BBBBATOM	3228	O	ASN	B	83	-5.086	-64.316	-30.472	1.00	21.92
BBBBATOM	3229	N	ALA	B	84	-3.203	-64.092	-29.275	1.00	19.74
BBBBATOM	3230	CA	ALA	B	84	-3.177	-62.647	-29.484	1.00	19.30
BBBBATOM	3231	CB	ALA	B	84	-2.060	-62.008	-28.662	1.00	18.59
BBBBATOM	3232	C	ALA	B	84	-2.967	-62.380	-30.981	1.00	19.94
BBBBATOM	3233	O	ALA	B	84	-3.561	-61.459	-31.552	1.00	19.69
BBBBATOM	3234	N	TRP	B	85	-2.118	-63.197	-31.603	1.00	19.77
BBBBATOM	3235	CA	TRP	B	85	-1.820	-63.111	-33.032	1.00	20.56
BBBBATOM	3236	CB	TRP	B	85	-0.754	-64.148	-33.396	1.00	21.46
BBBBATOM	3237	CG	TRP	B	85	-0.365	-64.167	-34.856	1.00	23.00
BBBBATOM	3238	CD2	TRP	B	85	-0.588	-65.232	-35.785	1.00	23.69
BBBBATOM	3239	CE2	TRP	B	85	-0.024	-64.835	-37.022	1.00	24.14
BBBBATOM	3240	CE3	TRP	B	85	-1.206	-66.486	-35.693	1.00	24.79
BBBBATOM	3241	CD1	TRP	B	85	0.301	-63.189	-35.548	1.00	23.17
BBBBATOM	3242	NE1	TRP	B	85	0.509	-63.585	-36.848	1.00	24.28
BBBBATOM	3243	CZ2	TRP	B	85	-0.060	-65.650	-38.160	1.00	24.90
BBBBATOM	3244	CZ3	TRP	B	85	-1.243	-67.299	-36.827	1.00	25.45
BBBBATOM	3245	CH2	TRP	B	85	-0.671	-66.875	-38.045	1.00	25.15
BBBBATOM	3246	C	TRP	B	85	-3.090	-63.354	-33.865	1.00	21.76
BBBBATOM	3247	O	TRP	B	85	-3.339	-62.658	-34.859	1.00	20.40
BBBBATOM	3248	N	ARG	B	86	-3.885	-64.346	-33.467	1.00	22.03
BBBBATOM	3249	CA	ARG	B	86	-5.140	-64.660	-34.166	1.00	23.28
BBBBATOM	3250	CB	ARG	B	86	-5.754	-65.965	-33.623	1.00	24.72
BBBBATOM	3251	CG	ARG	B	86	-4.999	-67.236	-34.021	1.00	27.21
BBBBATOM	3252	CD	ARG	B	86	-5.368	-67.725	-35.418	1.00	29.60
BBBBATOM	3253	NE	ARG	B	86	-6.626	-68.477	-35.422	1.00	31.45
BBBBATOM	3254	CZ	ARG	B	86	-7.185	-69.004	-36.508	1.00	31.37
BBBBATOM	3255	NH1	ARG	B	86	-6.607	-68.862	-37.696	1.00	32.19
BBBBATOM	3256	NH2	ARG	B	86	-8.314	-69.694	-36.405	1.00	31.39
BBBBATOM	3257	C	ARG	B	86	-6.151	-63.517	-34.007	1.00	22.98
BBBBATOM	3258	O	ARG	B	86	-6.890	-63.195	-34.942	1.00	21.37
BBBBATOM	3259	N	GLN	B	87	-6.190	-62.916	-32.821	1.00	22.90
BBBBATOM	3260	CA	GLN	B	87	-7.101	-61.802	-32.567	1.00	24.07

BBBBATOM	3261	CB	GLN	B	87	-7.046	-61.382	-31.097	1.00 24.33
BBBBATOM	3262	CG	GLN	B	87	-7.873	-62.280	-30.187	1.00 27.24
BBBBATOM	3263	CD	GLN	B	87	-7.720	-61.943	-28.723	1.00 28.81
BBBBATOM	3264	OE1	GLN	B	87	-8.567	-62.296	-27.908	1.00 33.25
BBBBATOM	3265	NE2	GLN	B	87	-6.632	-61.275	-28.375	1.00 29.95
BBBBATOM	3266	C	GLN	B	87	-6.738	-60.618	-33.457	1.00 23.85
BBBBATOM	3267	O	GLN	B	87	-7.613	-60.012	-34.077	1.00 24.02
BBBBATOM	3268	N	ALA	B	88	-5.449	-60.293	-33.521	1.00 23.39
BBBBATOM	3269	CA	ALA	B	88	-4.996	-59.183	-34.355	1.00 23.78
BBBBATOM	3270	CB	ALA	B	88	-3.508	-58.909	-34.116	1.00 23.33
BBBBATOM	3271	C	ALA	B	88	-5.257	-59.485	-35.831	1.00 24.73
BBBBATOM	3272	O	ALA	B	88	-5.655	-58.595	-36.592	1.00 24.72
BBBBATOM	3273	N	ARG	B	89	-5.038	-60.735	-36.244	1.00 24.26
BBBBATOM	3274	CA	ARG	B	89	-5.285	-61.111	-37.636	1.00 24.94
BBBBATOM	3275	CB	ARG	B	89	-4.904	-62.575	-37.893	1.00 25.14
BBBBATOM	3276	CG	ARG	B	89	-3.461	-62.774	-38.353	1.00 24.54
BBBBATOM	3277	CD	ARG	B	89	-3.142	-64.253	-38.510	1.00 25.50
BBBBATOM	3278	NE	ARG	B	89	-3.809	-64.901	-39.641	1.00 24.93
BBBBATOM	3279	CZ	ARG	B	89	-3.329	-64.930	-40.882	1.00 25.90
BBBBATOM	3280	NH1	ARG	B	89	-2.178	-64.336	-41.170	1.00 25.98
BBBBATOM	3281	NH2	ARG	B	89	-3.979	-65.596	-41.831	1.00 26.36
BBBBATOM	3282	C	ARG	B	89	-6.752	-60.909	-38.013	1.00 25.29
BBBBATOM	3283	O	ARG	B	89	-7.056	-60.420	-39.104	1.00 24.27
BBBBATOM	3284	N	ALA	B	90	-7.658	-61.296	-37.118	1.00 24.61
BBBBATOM	3285	CA	ALA	B	90	-9.088	-61.151	-37.383	1.00 26.16
BBBBATOM	3286	CB	ALA	B	90	-9.907	-61.775	-36.254	1.00 25.77
BBBBATOM	3287	C	ALA	B	90	-9.440	-59.673	-37.538	1.00 26.83
BBBBATOM	3288	O	ALA	B	90	-10.213	-59.301	-38.421	1.00 27.71
BBBBATOM	3289	N	ILE	B	91	-8.862	-58.837	-36.685	1.00 26.92
BBBBATOM	3290	CA	ILE	B	91	-9.108	-57.400	-36.733	1.00 26.97
BBBBATOM	3291	CB	ILE	B	91	-8.408	-56.682	-35.565	1.00 27.03
BBBBATOM	3292	CG2	ILE	B	91	-8.327	-55.175	-35.837	1.00 25.82
BBBBATOM	3293	CG1	ILE	B	91	-9.161	-56.962	-34.260	1.00 24.58
BBBBATOM	3294	CD1	ILE	B	91	-8.435	-56.490	-33.021	1.00 24.65
BBBBATOM	3295	C	ILE	B	91	-8.618	-56.787	-38.040	1.00 28.07
BBBBATOM	3296	O	ILE	B	91	-9.289	-55.934	-38.629	1.00 28.41
BBBBATOM	3297	N	MET	B	92	-7.451	-57.227	-38.496	1.00 27.92
BBBBATOM	3298	CA	MET	B	92	-6.872	-56.693	-39.717	1.00 29.03
BBBBATOM	3299	CB	MET	B	92	-5.366	-56.912	-39.712	1.00 27.34
BBBBATOM	3300	CG	MET	B	92	-4.686	-56.235	-38.536	1.00 26.09
BBBBATOM	3301	SD	MET	B	92	-2.919	-56.413	-38.602	1.00 25.72
BBBBATOM	3302	CE	MET	B	92	-2.413	-55.394	-37.218	1.00 24.09
BBBBATOM	3303	C	MET	B	92	-7.488	-57.257	-40.988	1.00 30.07
BBBBATOM	3304	O	MET	B	92	-7.417	-56.628	-42.046	1.00 30.66
BBBBATOM	3305	N	LYS	B	93	-8.082	-58.441	-40.894	1.00 30.96
BBBBATOM	3306	CA	LYS	B	93	-8.735	-59.038	-42.050	1.00 33.20
BBBBATOM	3307	CB	LYS	B	93	-8.969	-60.537	-41.826	1.00 34.31
BBBBATOM	3308	CG	LYS	B	93	-7.689	-61.369	-41.860	1.00 36.71
BBBBATOM	3309	CD	LYS	B	93	-7.956	-62.847	-41.576	1.00 38.43
BBBBATOM	3310	CE	LYS	B	93	-8.781	-63.491	-42.683	1.00 38.82
BBBBATOM	3311	NZ	LYS	B	93	-9.197	-64.881	-42.344	1.00 40.70
BBBBATOM	3312	C	LYS	B	93	-10.067	-58.314	-42.252	1.00 33.65
BBBBATOM	3313	O	LYS	B	93	-10.524	-58.143	-43.382	1.00 34.76
BBBBATOM	3314	N	ALA	B	94	-10.672	-57.877	-41.147	1.00 33.00
BBBBATOM	3315	CA	ALA	B	94	-11.943	-57.157	-41.183	1.00 33.62
BBBBATOM	3316	CB	ALA	B	94	-12.641	-57.260	-39.833	1.00 33.62
BBBBATOM	3317	C	ALA	B	94	-11.752	-55.684	-41.559	1.00 33.95
BBBBATOM	3318	O	ALA	B	94	-12.484	-55.153	-42.397	1.00 33.20
BBBBATOM	3319	N	TYR	B	95	-10.772	-55.028	-40.943	1.00 33.15
BBBBATOM	3320	CA	TYR	B	95	-10.504	-53.620	-41.224	1.00 33.83
BBBBATOM	3321	CB	TYR	B	95	-9.722	-52.992	-40.060	1.00 33.92
BBBBATOM	3322	CG	TYR	B	95	-9.383	-51.525	-40.249	1.00 34.38
BBBBATOM	3323	CD1	TYR	B	95	-10.381	-50.585	-40.499	1.00 36.04
BBBBATOM	3324	CE1	TYR	B	95	-10.071	-49.240	-40.702	1.00 36.49
BBBBATOM	3325	CD2	TYR	B	95	-8.063	-51.082	-40.202	1.00 34.89
BBBBATOM	3326	CE2	TYR	B	95	-7.741	-49.741	-40.401	1.00 35.72

BBBBATOM	3327	CZ	TYR	B	95	-8.750	-48.826	-40.655	1.00	36.79
BBBBATOM	3328	OH	TYR	B	95	-8.436	-47.562	-40.874	1.00	37.60
BBBBATOM	3329	C	TYR	B	95	-9.743	-53.418	-42.538	1.00	34.06
BBBBATOM	3330	O	TYR	B	95	-9.919	-52.404	-43.214	1.00	33.85
BBBBATOM	3331	N	LYS	B	96	-8.902	-54.386	-42.896	1.00	33.76
BBBBATOM	3332	CA	LYS	B	96	-8.104	-54.327	-44.122	1.00	33.85
BBBBATOM	3333	CB	LYS	B	96	-9.004	-54.476	-45.353	1.00	35.14
BBBBATOM	3334	CG	LYS	B	96	-9.707	-55.812	-45.463	1.00	37.16
BBBBATOM	3335	CD	LYS	B	96	-10.649	-55.843	-46.661	1.00	38.58
BBBBATOM	3336	CE	LYS	B	96	-11.388	-57.170	-46.752	1.00	40.07
BBBBATOM	3337	NZ	LYS	B	96	-12.319	-57.218	-47.925	1.00	41.29
BBBBATOM	3338	C	LYS	B	96	-7.278	-53.049	-44.262	1.00	33.75
BBBBATOM	3339	O	LYS	B	96	-7.489	-52.258	-45.189	1.00	34.55
BBBBATOM	3340	N	PRO	B	97	-6.326	-52.825	-43.345	1.00	32.59
BBBBATOM	3341	CD	PRO	B	97	-6.004	-53.620	-42.143	1.00	32.37
BBBBATOM	3342	CA	PRO	B	97	-5.490	-51.623	-43.419	1.00	31.82
BBBBATOM	3343	CB	PRO	B	97	-4.850	-51.568	-42.038	1.00	31.66
BBBBATOM	3344	CG	PRO	B	97	-4.686	-53.025	-41.704	1.00	31.53
BBBBATOM	3345	C	PRO	B	97	-4.458	-51.769	-44.530	1.00	31.60
BBBBATOM	3346	O	PRO	B	97	-4.052	-52.881	-44.860	1.00	32.52
BBBBATOM	3347	N	ASP	B	98	-4.037	-50.651	-45.112	1.00	31.25
BBBBATOM	3348	CA	ASP	B	98	-3.049	-50.685	-46.188	1.00	29.78
BBBBATOM	3349	CB	ASP	B	98	-3.234	-49.488	-47.117	1.00	32.00
BBBBATOM	3350	CG	ASP	B	98	-4.562	-49.519	-47.837	1.00	34.21
BBBBATOM	3351	OD1	ASP	B	98	-5.281	-48.498	-47.795	1.00	35.37
BBBBATOM	3352	OD2	ASP	B	98	-4.888	-50.566	-48.443	1.00	35.10
BBBBATOM	3353	C	ASP	B	98	-1.654	-50.660	-45.603	1.00	28.70
BBBBATOM	3354	O	ASP	B	98	-0.672	-50.973	-46.274	1.00	26.48
BBBBATOM	3355	N	VAL	B	99	-1.573	-50.278	-44.337	1.00	26.88
BBBBATOM	3356	CA	VAL	B	99	-0.296	-50.214	-43.660	1.00	26.75
BBBBATOM	3357	CB	VAL	B	99	0.500	-48.973	-44.132	1.00	27.35
BBBBATOM	3358	CG1	VAL	B	99	-0.305	-47.718	-43.867	1.00	29.45
BBBBATOM	3359	CG2	VAL	B	99	1.841	-48.908	-43.443	1.00	27.48
BBBBATOM	3360	C	VAL	B	99	-0.552	-50.134	-42.162	1.00	25.92
BBBBATOM	3361	O	VAL	B	99	-1.585	-49.627	-41.723	1.00	25.04
BBBBATOM	3362	N	VAL	B	100	0.374	-50.664	-41.377	1.00	24.63
BBBBATOM	3363	CA	VAL	B	100	0.227	-50.613	-39.936	1.00	23.59
BBBBATOM	3364	CB	VAL	B	100	0.120	-52.026	-39.327	1.00	24.97
BBBBATOM	3365	CG1	VAL	B	100	0.139	-51.941	-37.811	1.00	24.71
BBBBATOM	3366	CG2	VAL	B	100	-1.172	-52.683	-39.782	1.00	22.62
BBBBATOM	3367	C	VAL	B	100	1.428	-49.881	-39.382	1.00	22.74
BBBBATOM	3368	O	VAL	B	100	2.551	-50.093	-39.830	1.00	24.62
BBBBATOM	3369	N	LEU	B	101	1.178	-49.001	-38.419	1.00	21.89
BBBBATOM	3370	CA	LEU	B	101	2.214	-48.199	-37.797	1.00	21.59
BBBBATOM	3371	CB	LEU	B	101	1.823	-46.716	-37.853	1.00	22.86
BBBBATOM	3372	CG	LEU	B	101	2.850	-45.580	-37.892	1.00	24.72
BBBBATOM	3373	CD1	LEU	B	101	2.237	-44.385	-37.174	1.00	25.30
BBBBATOM	3374	CD2	LEU	B	101	4.168	-45.954	-37.273	1.00	24.45
BBBBATOM	3375	C	LEU	B	101	2.349	-48.604	-36.336	1.00	20.83
BBBBATOM	3376	O	LEU	B	101	1.370	-48.581	-35.595	1.00	21.35
BBBBATOM	3377	N	GLY	B	102	3.556	-48.986	-35.936	1.00	20.96
BBBBATOM	3378	CA	GLY	B	102	3.796	-49.357	-34.549	1.00	19.23
BBBBATOM	3379	C	GLY	B	102	4.655	-48.282	-33.918	1.00	18.45
BBBBATOM	3380	O	GLY	B	102	5.765	-48.016	-34.381	1.00	18.70
BBBBATOM	3381	N	MET	B	103	4.155	-47.660	-32.857	1.00	18.01
BBBBATOM	3382	CA	MET	B	103	4.892	-46.597	-32.191	1.00	18.93
BBBBATOM	3383	CB	MET	B	103	3.928	-45.477	-31.781	1.00	20.02
BBBBATOM	3384	CG	MET	B	103	3.121	-44.888	-32.944	1.00	21.61
BBBBATOM	3385	SD	MET	B	103	4.212	-44.135	-34.157	1.00	23.45
BBBBATOM	3386	CE	MET	B	103	4.718	-42.680	-33.271	1.00	21.40
BBBBATOM	3387	C	MET	B	103	5.612	-47.128	-30.957	1.00	18.98
BBBBATOM	3388	O	MET	B	103	6.134	-46.357	-30.158	1.00	17.96
BBBBATOM	3389	N	GLY	B	104	5.640	-48.450	-30.827	1.00	21.56
BBBBATOM	3390	CA	GLY	B	104	6.275	-49.080	-29.686	1.00	21.89
BBBBATOM	3391	C	GLY	B	104	5.192	-49.614	-28.764	1.00	23.28
BBBBATOM	3392	O	GLY	B	104	4.009	-49.353	-28.980	1.00	22.50

BBBBATOM	3393	N	GLY	B	105	5.583	-50.364	-27.741	1.00 23.01
BBBBATOM	3394	CA	GLY	B	105	4.593	-50.965	-26.827	1.00 23.54
BBBBATOM	3395	C	GLY	B	105	4.358	-52.380	-27.078	1.00 23.17
BBBBATOM	3396	O	GLY	B	105	4.449	-52.844	-28.214	1.00 22.69
BBBBATOM	3397	N	TYR	B	106	4.018	-53.118	-26.026	1.00 22.87
BBBBATOM	3398	CA	TYR	B	106	3.818	-54.554	-26.159	1.00 22.37
BBBBATOM	3399	CB	TYR	B	106	3.632	-55.181	-24.774	1.00 25.08
BBBBATOM	3400	CG	TYR	B	106	4.864	-55.008	-23.929	1.00 28.19
BBBBATOM	3401	CD1	TYR	B	106	4.869	-54.153	-22.830	1.00 31.96
BBBBATOM	3402	CE1	TYR	B	106	6.043	-53.915	-22.108	1.00 33.13
BBBBATOM	3403	CD2	TYR	B	106	6.058	-55.631	-24.282	1.00 31.27
BBBBATOM	3404	CE2	TYR	B	106	7.234	-55.400	-23.569	1.00 32.27
BBBBATOM	3405	CZ	TYR	B	106	7.219	-54.541	-22.487	1.00 33.19
BBBBATOM	3406	OH	TYR	B	106	8.388	-54.291	-21.802	1.00 35.95
BBBBATOM	3407	C	TYR	B	106	2.719	-55.018	-27.100	1.00 20.52
BBBBATOM	3408	O	TYR	B	106	2.867	-56.052	-27.746	1.00 20.50
BBBBATOM	3409	N	VAL	B	107	1.628	-54.270	-27.205	1.00 19.06
BBBBATOM	3410	CA	VAL	B	107	0.557	-54.694	-28.099	1.00 18.06
BBBBATOM	3411	CB	VAL	B	107	-0.690	-53.774	-27.978	1.00 20.95
BBBBATOM	3412	CG1	VAL	B	107	-0.407	-52.407	-28.589	1.00 21.39
BBBBATOM	3413	CG2	VAL	B	107	-1.879	-54.433	-28.658	1.00 21.30
BBBBATOM	3414	C	VAL	B	107	1.015	-54.743	-29.559	1.00 17.45
BBBBATOM	3415	O	VAL	B	107	0.502	-55.536	-30.346	1.00 16.99
BBBBATOM	3416	N	SER	B	108	1.991	-53.916	-29.918	1.00 17.96
BBBBATOM	3417	CA	SER	B	108	2.488	-53.892	-31.290	1.00 19.67
BBBBATOM	3418	CB	SER	B	108	3.424	-52.691	-31.508	1.00 19.56
BBBBATOM	3419	OG	SER	B	108	4.666	-52.824	-30.837	1.00 19.63
BBBBATOM	3420	C	SER	B	108	3.197	-55.187	-31.694	1.00 20.38
BBBBATOM	3421	O	SER	B	108	3.385	-55.449	-32.884	1.00 21.25
BBBBATOM	3422	N	GLY	B	109	3.595	-55.995	-30.710	1.00 19.59
BBBBATOM	3423	CA	GLY	B	109	4.251	-57.256	-31.023	1.00 20.03
BBBBATOM	3424	C	GLY	B	109	3.311	-58.170	-31.792	1.00 19.61
BBBBATOM	3425	O	GLY	B	109	3.579	-58.517	-32.940	1.00 19.24
BBBBATOM	3426	N	PRO	B	110	2.206	-58.606	-31.173	1.00 19.20
BBBBATOM	3427	CD	PRO	B	110	1.914	-58.528	-29.729	1.00 19.94
BBBBATOM	3428	CA	PRO	B	110	1.251	-59.478	-31.855	1.00 18.99
BBBBATOM	3429	CB	PRO	B	110	0.198	-59.737	-30.778	1.00 20.41
BBBBATOM	3430	CG	PRO	B	110	0.998	-59.720	-29.515	1.00 19.81
BBBBATOM	3431	C	PRO	B	110	0.651	-58.761	-33.075	1.00 19.22
BBBBATOM	3432	O	PRO	B	110	0.406	-59.371	-34.116	1.00 17.13
BBBBATOM	3433	N	GLY	B	111	0.407	-57.462	-32.927	1.00 19.03
BBBBATOM	3434	CA	GLY	B	111	-0.160	-56.702	-34.025	1.00 19.60
BBBBATOM	3435	C	GLY	B	111	0.764	-56.714	-35.226	1.00 19.59
BBBBATOM	3436	O	GLY	B	111	0.330	-56.979	-36.339	1.00 21.10
BBBBATOM	3437	N	GLY	B	112	2.043	-56.429	-34.995	1.00 19.78
BBBBATOM	3438	CA	GLY	B	112	3.014	-56.417	-36.074	1.00 19.97
BBBBATOM	3439	C	GLY	B	112	3.147	-57.783	-36.724	1.00 20.43
BBBBATOM	3440	O	GLY	B	112	3.233	-57.896	-37.949	1.00 19.94
BBBBATOM	3441	N	LEU	B	113	3.167	-58.828	-35.903	1.00 19.26
BBBBATOM	3442	CA	LEU	B	113	3.265	-60.184	-36.429	1.00 19.49
BBBBATOM	3443	CB	LEU	B	113	3.405	-61.198	-35.289	1.00 18.38
BBBBATOM	3444	CG	LEU	B	113	4.777	-61.270	-34.605	1.00 20.59
BBBBATOM	3445	CD1	LEU	B	113	4.656	-62.059	-33.311	1.00 20.01
BBBBATOM	3446	CD2	LEU	B	113	5.794	-61.914	-35.538	1.00 20.23
BBBBATOM	3447	C	LEU	B	113	2.040	-60.521	-37.274	1.00 18.73
BBBBATOM	3448	O	LEU	B	113	2.143	-61.252	-38.255	1.00 18.44
BBBBATOM	3449	N	ALA	B	114	0.875	-60.010	-36.892	1.00 18.96
BBBBATOM	3450	CA	ALA	B	114	-0.334	-60.292	-37.661	1.00 18.70
BBBBATOM	3451	CB	ALA	B	114	-1.562	-59.855	-36.889	1.00 16.45
BBBBATOM	3452	C	ALA	B	114	-0.288	-59.578	-39.019	1.00 19.30
BBBBATOM	3453	O	ALA	B	114	-0.602	-60.167	-40.052	1.00 20.62
BBBBATOM	3454	N	ALA	B	115	0.082	-58.303	-39.000	1.00 20.57
BBBBATOM	3455	CA	ALA	B	115	0.167	-57.516	-40.229	1.00 21.84
BBBBATOM	3456	CB	ALA	B	115	0.636	-56.108	-39.911	1.00 19.85
BBBBATOM	3457	C	ALA	B	115	1.140	-58.192	-41.189	1.00 21.58
BBBBATOM	3458	O	ALA	B	115	0.815	-58.464	-42.345	1.00 22.14

BBBBATOM	3459	N	TRP	B	116	2.334	-58.476	-40.688	1.00 22.12
BBBBATOM	3460	CA	TRP	B	116	3.365	-59.426	-41.478	1.00 23.22
BBBBATOM	3461	CB	TRP	B	116	4.584	-59.367	-40.579	1.00 26.08
BBBBATOM	3462	CG	TRP	B	116	5.699	-60.136	-41.204	1.00 27.40
BBBBATOM	3463	CD2	TRP	B	116	6.168	-61.418	-40.793	1.00 28.77
BBBBATOM	3464	CE2	TRP	B	116	7.234	-61.771	-41.655	1.00 30.37
BBBBATOM	3465	CE3	TRP	B	116	5.794	-62.308	-39.778	1.00 30.49
BBBBATOM	3466	CD1	TRP	B	116	6.473	-59.761	-42.271	1.00 28.30
BBBBATOM	3467	NE1	TRP	B	116	7.401	-60.742	-42.547	1.00 29.04
BBBBATOM	3468	CZ2	TRP	B	116	7.929	-62.981	-41.529	1.00 31.08
BBBBATOM	3469	CZ3	TRP	B	116	6.485	-63.510	-39.653	1.00 31.85
BBBBATOM	3470	CH2	TRP	B	116	7.541	-63.834	-40.527	1.00 32.27
BBBBATOM	3471	C	TRP	B	116	2.871	-60.434	-42.123	1.00 23.55
BBBBATOM	3472	O	TRP	B	116	3.048	-60.643	-43.329	1.00 22.19
BBBBATOM	3473	N	SER	B	117	2.231	-61.304	-41.338	1.00 21.35
BBBBATOM	3474	CA	SER	B	117	1.735	-62.573	-41.873	1.00 22.61
BBBBATOM	3475	CB	SER	B	117	1.167	-63.462	-40.756	1.00 20.72
BBBBATOM	3476	OG	SER	B	117	0.010	-62.889	-40.169	1.00 22.72
BBBBATOM	3477	C	SER	B	117	0.665	-62.383	-42.940	1.00 23.56
BBBBATOM	3478	O	SER	B	117	0.463	-63.262	-43.780	1.00 23.11
BBBBATOM	3479	N	LEU	B	118	-0.020	-61.242	-42.905	1.00 24.40
BBBBATOM	3480	CA,	LEU	B	118	-1.069	-60.957	-43.882	1.00 25.70
BBBBATOM	3481	CB	LEU	B	118	-2.195	-60.155	-43.227	1.00 25.80
BBBBATOM	3482	CG	LEU	B	118	-3.012	-60.889	-42.159	1.00 26.56
BBBBATOM	3483	CD1	LEU	B	118	-3.905	-59.895	-41.433	1.00 26.62
BBBBATOM	3484	CD2	LEU	B	118	-3.841	-62.000	-42.801	1.00 26.51
BBBBATOM	3485	C	LEU	B	118	-0.539	-60.193	-45.094	1.00 26.87
BBBBATOM	3486	O	LEU	B	118	-1.292	-59.878	-46.021	1.00 26.69
BBBBATOM	3487	N	GLY	B	119	0.755	-59.898	-45.085	1.00 26.39
BBBBATOM	3488	CA	GLY	B	119	1.354	-59.174	-46.192	1.00 27.80
BBBBATOM	3489	C	GLY	B	119	1.142	-57.671	-46.120	1.00 27.64
BBBBATOM	3490	O	GLY	B	119	1.293	-56.972	-47.122	1.00 28.49
BBBBATOM	3491	N	ILE	B	120	0.786	-57.173	-44.940	1.00 25.88
BBBBATOM	3492	CA	ILE	B	120	0.568	-55.744	-44.731	1.00 24.85
BBBBATOM	3493	CB	ILE	B	120	-0.507	-55.497	-43.652	1.00 24.64
BBBBATOM	3494	CG2	ILE	B	120	-0.648	-54.000	-43.397	1.00 24.49
BBBBATOM	3495	CG1	ILE	B	120	-1.839	-56.112	-44.093	1.00 24.61
BBBBATOM	3496	CD1	ILE	B	120	-2.891	-56.170	-42.991	1.00 23.34
BBBBATOM	3497	C	ILE	B	120	1.879	-55.121	-44.272	1.00 24.55
BBBBATOM	3498	O	ILE	B	120	2.465	-55.551	-43.275	1.00 23.69
BBBBATOM	3499	N	PRO	B	121	2.365	-54.098	-44.995	1.00 23.85
BBBBATOM	3500	CD	PRO	B	121	1.780	-53.400	-46.154	1.00 23.64
BBBBATOM	3501	CA	PRO	B	121	3.625	-53.477	-44.591	1.00 22.63
BBBBATOM	3502	CB	PRO	B	121	3.872	-52.440	-45.691	1.00 23.83
BBBBATOM	3503	CG	PRO	B	121	2.485	-52.053	-46.102	1.00 23.96
BBBBATOM	3504	C	PRO	B	121	3.583	-52.869	-43.196	1.00 22.21
BBBBATOM	3505	O	PRO	B	121	2.617	-52.208	-42.810	1.00 22.46
BBBBATOM	3506	N	VAL	B	122	4.641	-53.114	-42.437	1.00 21.69
BBBBATOM	3507	CA	VAL	B	122	4.743	-52.594	-41.083	1.00 22.03
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BBBBATOM	3509	CG1	VAL	B	122	5.426	-53.085	-38.724	1.00 21.97
BBBBATOM	3510	CG2	VAL	B	122	4.133	-54.789	-40.035	1.00 22.19
BBBBATOM	3511	C	VAL	B	122	5.754	-51.465	-41.021	1.00 21.29
BBBBATOM	3512	O	VAL	B	122	6.892	-51.605	-41.479	1.00 22.83
BBBBATOM	3513	N	VAL	B	123	5.330	-50.338	-40.464	1.00 20.94
BBBBATOM	3514	CA	VAL	B	123	6.200	-49.184	-40.310	1.00 20.82
BBBBATOM	3515	CB	VAL	B	123	5.580	-47.902	-40.932	1.00 22.16
BBBBATOM	3516	CG1	VAL	B	123	6.516	-46.722	-40.709	1.00 20.83
BBBBATOM	3517	CG2	VAL	B	123	5.322	-48.111	-42.420	1.00 22.66
BBBBATOM	3518	C	VAL	B	123	6.338	-48.953	-38.812	1.00 21.09
BBBBATOM	3519	O	VAL	B	123	5.341	-48.986	-38.093	1.00 21.48
BBBBATOM	3520	N	LEU	B	124	7.557	-48.720	-38.340	1.00 20.53
BBBBATOM	3521	CA	LEU	B	124	7.749	-48.485	-36.915	1.00 22.10
BBBBATOM	3522	CB	LEU	B	124	8.578	-49.606	-36.286	1.00 22.00
BBBBATOM	3523	CG	LEU	B	124	8.160	-51.051	-36.551	1.00 22.45
BBBBATOM	3524	CD1	LEU	B	124	9.196	-51.974	-35.905	1.00 23.90

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BBBBATOM   3525  CD2 LEU B 124      6.765 -51.313 -36.003  1.00 22.34
BBBBATOM   3526  C   LEU B 124      8.452 -47.472 -36.633  1.00 22.36
BBBBATOM   3527  O   LEU B 124      9.218 -46.660 -37.461  1.00 20.75
BBBBATOM   3528  N   HIS B 125      8.182 -46.638 -35.447  1.00 21.40
BBBBATOM   3529  CA  HIS B 125      8.814 -45.413 -34.981  1.00 21.42
BBBBATOM   3530  CB  HIS B 125      7.858 -44.218 -35.067  1.00 21.57
BBBBATOM   3531  CG  HIS B 125      8.432 -42.948 -34.511  1.00 23.73
BBBBATOM   3532  CD2 HIS B 125      8.300 -42.368 -33.295  1.00 22.15
BBBBATOM   3533  ND1 HIS B 125      9.274 -42.127 -35.236  1.00 26.23
BBBBATOM   3534  CE1 HIS B 125      9.631 -41.095 -34.490  1.00 24.20
BBBBATOM   3535  NE2 HIS B 125      9.054 -41.218 -33.307  1.00 26.07
BBBBATOM   3536  C   HIS B 125      9.196 -45.642 -33.519  1.00 21.70
BBBBATOM   3537  O   HIS B 125      8.378 -46.117 -32.725  1.00 19.81
BBBBATOM   3538  N   GLU B 126     10.444 -45.332 -33.186  1.00 21.20
BBBBATOM   3539  CA  GLU B 126     10.947 -45.452 -31.817  1.00 22.15
BBBBATOM   3540  CB  GLU B 126     12.252 -46.246 -31.790  1.00 21.99
BBBBATOM   3541  CG  GLU B 126     12.958 -46.206 -30.439  1.00 22.04
BBBBATOM   3542  CD  GLU B 126     12.119 -46.824 -29.338  1.00 21.43
BBBBATOM   3543  OE1 GLU B 126     11.767 -48.014 -29.471  1.00 21.92
BBBBATOM   3544  OE2 GLU B 126     11.807 -46.124 -28.349  1.00 21.08
BBBBATOM   3545  C   GLU B 126     11.205 -44.027 -31.326  1.00 21.93
BBBBATOM   3546  O   GLU B 126     12.016 -43.300 -31.908  1.00 21.33
BBBBATOM   3547  N   GLN B 127     10.520 -43.624 -30.259  1.00 22.62
BBBBATOM   3548  CA  GLN B 127     10.682 -42.270 -29.735  1.00 22.81
BBBBATOM   3549  CB  GLN B 127      9.414 -41.814 -28.989  1.00 23.56
BBBBATOM   3550  CG  GLN B 127      8.147 -41.783 -29.830  1.00 24.46
BBBBATOM   3551  CD  GLN B 127      7.312 -43.041 -29.687  1.00 25.85
BBBBATOM   3552  OE1 GLN B 127      6.842 -43.366 -28.591  1.00 23.78
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BBBBATOM   3554  C   GLN B 127     11.874 -42.087 -28.809  1.00 22.39
BBBBATOM   3555  O   GLN B 127     12.399 -40.976 -28.682  1.00 22.43
BBBBATOM   3556  N   ASN B 128     12.314 -43.173 -28.177  1.00 22.35
BBBBATOM   3557  CA  ASN B 128     13.406 -43.097 -27.216  1.00 22.96
BBBBATOM   3558  CB  ASN B 128     13.136 -44.080 -26.064  1.00 22.85
BBBBATOM   3559  CG  ASN B 128     11.742 -43.919 -25.474  1.00 23.25
BBBBATOM   3560  OD1 ASN B 128     10.804 -44.632 -25.848  1.00 26.04
BBBBATOM   3561  ND2 ASN B 128     11.597 -42.975 -24.556  1.00 22.68
BBBBATOM   3562  C   ASN B 128     14.824 -43.314 -27.742  1.00 23.87
BBBBATOM   3563  O   ASN B 128     15.026 -43.856 -28.830  1.00 24.05
BBBBATOM   3564  N   GLY B 129     15.798 -42.885 -26.940  1.00 24.35
BBBBATOM   3565  CA  GLY B 129     17.203 -43.019 -27.294  1.00 25.36
BBBBATOM   3566  C   GLY B 129     17.642 -44.468 -27.280  1.00 25.97
BBBBATOM   3567  O   GLY B 129     18.643 -44.836 -27.891  1.00 25.48
BBBBATOM   3568  N   ILE B 130     16.886 -45.290 -26.565  1.00 26.18
BBBBATOM   3569  CA  ILE B 130     17.160 -46.716 -26.488  1.00 28.00
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BBBBATOM   3571  CG2 ILE B 130     16.323 -46.785 -24.102  1.00 28.52
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BBBBATOM   3573  CD1 ILE B 130     18.097 -49.149 -23.593  1.00 31.39
BBBBATOM   3574  C   ILE B 130     15.909 -47.435 -26.999  1.00 27.44
BBBBATOM   3575  O   ILE B 130     14.793 -47.103 -26.610  1.00 28.58
BBBBATOM   3576  N   ALA B 131     16.097 -48.405 -27.887  1.00 26.98
BBBBATOM   3577  CA  ALA B 131     14.978 -49.139 -28.461  1.00 25.88
BBBBATOM   3578  CB  ALA B 131     15.485 -50.102 -29.525  1.00 25.02
BBBBATOM   3579  C   ALA B 131     14.171 -49.901 -27.413  1.00 25.20
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BBBBATOM   3581  N   GLY B 132     12.851 -49.814 -27.506  1.00 24.52
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BBBBATOM   3583  C   GLY B 132     12.150 -52.019 -26.831  1.00 23.35
BBBBATOM   3584  O   GLY B 132     12.582 -52.419 -27.904  1.00 22.89
BBBBATOM   3585  N   LEU B 133     11.788 -52.846 -25.860  1.00 23.38
BBBBATOM   3586  CA  LEU B 133     11.903 -54.293 -26.020  1.00 24.54
BBBBATOM   3587  CB  LEU B 133     11.328 -54.996 -24.786  1.00 25.48
BBBBATOM   3588  CG  LEU B 133     11.388 -56.527 -24.780  1.00 27.50
BBBBATOM   3589  CD1 LEU B 133     12.840 -56.984 -24.866  1.00 28.69
BBBBATOM   3590  CD2 LEU B 133     10.735 -57.059 -23.509  1.00 28.04
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BBBBATOM	3591	C	LEU	B	133	11.209	-54.833	-27.276	1.00	22.84
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BBBBATOM	3593	N	THR	B	134	9.975	-54.401	-27.499	1.00	21.72
BBBBATOM	3594	CA	THR	B	134	9.202	-54.860	-28.639	1.00	21.22
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BBBBATOM	3597	CG2	THR	B	134	6.872	-55.073	-29.600	1.00	20.64
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BBBBATOM	3610	CB	LYS	B	136	14.713	-54.196	-29.879	1.00	24.70
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BBBBATOM	3612	CD	LYS	B	136	16.998	-54.494	-28.902	1.00	30.17
BBBBATOM	3613	CE	LYS	B	136	18.479	-54.671	-29.203	1.00	32.33
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BBBBATOM	3615	C	LYS	B	136	13.793	-55.229	-31.966	1.00	23.46
BBBBATOM	3616	O	LYS	B	136	14.561	-55.407	-32.912	1.00	23.71
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BBBBATOM	3619	CB	TRP	B	137	12.361	-58.552	-31.553	1.00	21.20
BBBBATOM	3620	CG	TRP	B	137	10.990	-58.525	-30.922	1.00	20.23
BBBBATOM	3621	CD2	TRP	B	137	9.748	-58.877	-31.544	1.00	18.68
BBBBATOM	3622	CE2	TRP	B	137	8.743	-58.780	-30.555	1.00	18.97
BBBBATOM	3623	CE3	TRP	B	137	9.383	-59.270	-32.840	1.00	19.75
BBBBATOM	3624	CD1	TRP	B	137	10.696	-58.231	-29.618	1.00	19.62
BBBBATOM	3625	NE1	TRP	B	137	9.349	-58.385	-29.390	1.00	19.31
BBBBATOM	3626	CZ2	TRP	B	137	7.401	-59.058	-30.821	1.00	18.18
BBBBATOM	3627	CZ3	TRP	B	137	8.046	-59.549	-33.107	1.00	18.87
BBBBATOM	3628	CH2	TRP	B	137	7.072	-59.440	-32.099	1.00	18.94
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BBBBATOM	3631	N	LEU	B	138	10.741	-56.381	-33.386	1.00	21.61
BBBBATOM	3632	CA	LEU	B	138	9.744	-56.188	-34.431	1.00	23.15
BBBBATOM	3633	CB	LEU	B	138	8.618	-55.305	-33.886	1.00	23.87
BBBBATOM	3634	CG	LEU	B	138	7.312	-55.155	-34.664	1.00	26.48
BBBBATOM	3635	CD1	LEU	B	138	6.672	-56.508	-34.915	1.00	25.34
BBBBATOM	3636	CD2	LEU	B	138	6.383	-54.267	-33.851	1.00	25.90
BBBBATOM	3637	C	LEU	B	138	10.384	-55.558	-35.676	1.00	23.07
BBBBATOM	3638	O	LEU	B	138	9.958	-55.801	-36.809	1.00	22.68
BBBBATOM	3639	N	ALA	B	139	11.423	-54.763	-35.453	1.00	23.34
BBBBATOM	3640	CA	ALA	B	139	12.128	-54.092	-36.542	1.00	25.29
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BBBBATOM	3642	C	ALA	B	139	12.624	-55.064	-37.610	1.00	26.83
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BBBBATOM	3644	N	LYS	B	140	12.801	-56.332	-37.241	1.00	27.38
BBBBATOM	3645	CA	LYS	B	140	13.279	-57.337	-38.182	1.00	28.05
BBBBATOM	3646	CB	LYS	B	140	13.893	-58.501	-37.401	1.00	29.91
BBBBATOM	3647	CG	LYS	B	140	15.134	-58.057	-36.635	1.00	31.62
BBBBATOM	3648	CD	LYS	B	140	15.719	-59.149	-35.757	1.00	33.53
BBBBATOM	3649	CE	LYS	B	140	16.974	-58.634	-35.055	1.00	34.46
BBBBATOM	3650	NZ	LYS	B	140	17.692	-59.713	-34.320	1.00	36.17
BBBBATOM	3651	C	LYS	B	140	12.254	-57.833	-39.212	1.00	27.83
BBBBATOM	3652	O	LYS	B	140	12.602	-58.562	-40.142	1.00	27.80
BBBBATOM	3653	N	ILE	B	141	10.992	-57.445	-39.052	1.00	26.40
BBBBATOM	3654	CA	ILE	B	141	9.963	-57.818	-40.016	1.00	26.09
BBBBATOM	3655	CB	ILE	B	141	8.854	-58.721	-39.405	1.00	26.39
BBBBATOM	3656	CG2	ILE	B	141	9.401	-60.118	-39.145	1.00	28.33

BBBBATOM	3657	CG1	ILE	B	141	8.298	-58.092	-38.127	1.00	26.45
BBBBATOM	3658	CD1	ILE	B	141	7.136	-58.845	-37.549	1.00	26.95
BBBBATOM	3659	C	ILE	B	141	9.316	-56.542	-40.530	1.00	25.81
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BBBBATOM	3661	N	ALA	B	142	9.856	-55.405	-40.097	1.00	23.78
BBBBATOM	3662	CA	ALA	B	142	9.331	-54.107	-40.498	1.00	25.03
BBBBATOM	3663	CB	ALA	B	142	9.717	-53.046	-39.466	1.00	24.89
BBBBATOM	3664	C	ALA	B	142	9.816	-53.680	-41.880	1.00	25.08
BBBBATOM	3665	O	ALA	B	142	10.973	-53.894	-42.237	1.00	24.93
BBBBATOM	3666	N	THR	B	143	8.920	-53.075	-42.651	1.00	25.03
BBBBATOM	3667	CA	THR	B	143	9.262	-52.595	-43.984	1.00	26.10
BBBBATOM	3668	CB	THR	B	143	7.987	-52.318	-44.816	1.00	25.75
BBBBATOM	3669	OG1	THR	B	143	7.249	-53.534	-44.970	1.00	25.54
BBBBATOM	3670	CG2	THR	B	143	8.345	-51.782	-46.207	1.00	26.92
BBBBATOM	3671	C	THR	B	143	10.079	-51.310	-43.863	1.00	26.63
BBBBATOM	3672	O	THR	B	143	10.996	-51.061	-44.656	1.00	27.13
BBBBATOM	3673	N	LYS	B	144	9.753	-50.506	-42.853	1.00	24.95
BBBBATOM	3674	CA	LYS	B	144	10.436	-49.238	-42.618	1.00	24.73
BBBBATOM	3675	CB	LYS	B	144	9.688	-48.103	-43.329	1.00	26.20
BBBBATOM	3676	CG	LYS	B	144	10.202	-46.710	-43.013	1.00	27.44
BBBBATOM	3677	CD	LYS	B	144	11.602	-46.480	-43.558	1.00	29.01
BBBBATOM	3678	CE	LYS	B	144	12.055	-45.051	-43.293	1.00	29.74
BBBBATOM	3679	NZ	LYS	B	144	13.406	-44.774	-43.854	1.00	31.29
BBBBATOM	3680	C	LYS	B	144	10.506	-48.943	-41.125	1.00	24.61
BBBBATOM	3681	O	LYS	B	144	9.493	-49.008	-40.423	1.00	23.36
BBBBATOM	3682	N	VAL	B	145	11.707	-48.623	-40.656	1.00	23.68
BBBBATOM	3683	CA	VAL	B	145	11.947	-48.311	-39.252	1.00	23.62
BBBBATOM	3684	CB	VAL	B	145	12.981	-49.279	-38.617	1.00	23.66
BBBBATOM	3685	CG1	VAL	B	145	13.083	-49.014	-37.114	1.00	24.44
BBBBATOM	3686	CG2	VAL	B	145	12.589	-50.724	-38.878	1.00	23.51
BBBBATOM	3687	C	VAL	B	145	12.510	-46.900	-39.125	1.00	24.09
BBBBATOM	3688	O	VAL	B	145	13.473	-46.545	-39.808	1.00	23.68
BBBBATOM	3689	N	MET	B	146	11.902	-46.103	-38.251	1.00	23.84
BBBBATOM	3690	CA	MET	B	146	12.338	-44.736	-37.993	1.00	23.15
BBBBATOM	3691	CB	MET	B	146	11.274	-43.729	-38.448	1.00	24.72
BBBBATOM	3692	CG	MET	B	146	11.130	-43.577	-39.970	1.00	21.76
BBBBATOM	3693	SD	MET	B	146	9.649	-42.636	-40.468	1.00	25.05
BBBBATOM	3694	CE	MET	B	146	8.376	-43.846	-40.325	1.00	21.96
BBBBATOM	3695	C	MET	B	146	12.567	-44.593	-36.488	1.00	24.69
BBBBATOM	3696	O	MET	B	146	11.963	-45.311	-35.689	1.00	22.43
BBBBATOM	3697	N	GLN	B	147	13.456	-43.678	-36.112	1.00	23.37
BBBBATOM	3698	CA	GLN	B	147	13.762	-43.418	-34.712	1.00	25.05
BBBBATOM	3699	CB	GLN	B	147	15.067	-44.114	-34.301	1.00	24.99
BBBBATOM	3700	CG	GLN	B	147	16.259	-43.750	-35.169	1.00	26.10
BBBBATOM	3701	CD	GLN	B	147	17.527	-44.508	-34.803	1.00	26.65
BBBBATOM	3702	OE1	GLN	B	147	18.425	-44.671	-35.637	1.00	28.62
BBBBATOM	3703	NE2	GLN	B	147	17.615	-44.966	-33.558	1.00	26.05
BBBBATOM	3704	C	GLN	B	147	13.880	-41.911	-34.515	1.00	26.28
BBBBATOM	3705	O	GLN	B	147	14.292	-41.177	-35.430	1.00	25.02
BBBBATOM	3706	N	ALA	B	148	13.518	-41.452	-33.323	1.00	26.58
BBBBATOM	3707	CA	ALA	B	148	13.559	-40.032	-33.009	1.00	26.88
BBBBATOM	3708	CB	ALA	B	148	12.853	-39.776	-31.685	1.00	26.71
BBBBATOM	3709	C	ALA	B	148	14.983	-39.502	-32.954	1.00	27.88
BBBBATOM	3710	O	ALA	B	148	15.293	-38.463	-33.545	1.00	27.38
BBBBATOM	3711	N	PHE	B	149	15.847	-40.219	-32.242	1.00	27.92
BBBBATOM	3712	CA	PHE	B	149	17.239	-39.820	-32.098	1.00	29.39
BBBBATOM	3713	CB	PHE	B	149	17.596	-39.631	-30.617	1.00	28.95
BBBBATOM	3714	CG	PHE	B	149	16.549	-38.910	-29.821	1.00	28.91
BBBBATOM	3715	CD1	PHE	B	149	15.745	-39.603	-28.929	1.00	27.96
BBBBATOM	3716	CD2	PHE	B	149	16.372	-37.537	-29.957	1.00	29.03
BBBBATOM	3717	CE1	PHE	B	149	14.779	-38.945	-28.178	1.00	28.64
BBBBATOM	3718	CE2	PHE	B	149	15.406	-36.866	-29.211	1.00	30.10
BBBBATOM	3719	CZ	PHE	B	149	14.608	-37.575	-28.317	1.00	29.02
BBBBATOM	3720	C	PHE	B	149	18.153	-40.893	-32.673	1.00	30.03
BBBBATOM	3721	O	PHE	B	149	17.750	-42.036	-32.849	1.00	30.05
BBBBATOM	3722	N	PRO	B	150	19.401	-40.530	-32.991	1.00	31.73

BBBBATOM	3723	CD	PRO	B	150	20.018	-39.192	-33.018	1.00	32.39
BBBBATOM	3724	CA	PRO	B	150	20.310	-41.641	-33.535	1.00	31.87
BBBBATOM	3725	CB	PRO	B	150	21.418	-40.698	-34.154	1.00	33.07
BBBBATOM	3726	CG	PRO	B	150	21.480	-39.517	-33.238	1.00	33.70
BBBBATOM	3727	C	PRO	B	150	20.809	-42.411	-32.376	1.00	31.93
BBBBATOM	3728	O	PRO	B	150	20.873	-41.945	-31.239	1.00	31.39
BBBBATOM	3729	N	GLY	B	151	21.130	-43.671	-32.651	1.00	31.67
BBBBATOM	3730	CA	GLY	B	151	21.629	-44.537	-31.595	1.00	32.62
BBBBATOM	3731	C	GLY	B	151	20.717	-45.655	-31.112	1.00	32.88
BBBBATOM	3732	O	GLY	B	151	21.206	-46.690	-30.657	1.00	32.98
BBBBATOM	3733	N	ALA	B	152	19.403	-45.458	-31.196	1.00	32.24
BBBBATOM	3734	CA	ALA	B	152	18.447	-46.476	-30.753	1.00	32.71
BBBBATOM	3735	CB	ALA	B	152	17.020	-45.924	-30.817	1.00	31.78
BBBBATOM	3736	C	ALA	B	152	18.582	-47.708	-31.643	1.00	33.00
BBBBATOM	3737	O	ALA	B	152	18.528	-48.842	-31.169	1.00	32.08
BBBBATOM	3738	N	PHE	B	153	18.732	-47.462	-32.941	1.00	33.66
BBBBATOM	3739	CA	PHE	B	153	18.925	-48.506	-33.937	1.00	34.83
BBBBATOM	3740	CB	PHE	B	153	17.734	-48.611	-34.893	1.00	33.64
BBBBATOM	3741	CG	PHE	B	153	16.518	-49.244	-34.289	1.00	32.97
BBBBATOM	3742	CD1	PHE	B	153	15.468	-48.461	-33.823	1.00	31.93
BBBBATOM	3743	CD2	PHE	B	153	16.421	-50.628	-34.184	1.00	32.46
BBBBATOM	3744	CE1	PHE	B	153	14.339	-49.049	-33.265	1.00	32.18
BBBBATOM	3745	CE2	PHE	B	153	15.294	-51.224	-33.626	1.00	31.75
BBBBATOM	3746	CZ	PHE	B	153	14.254	-50.435	-33.166	1.00	31.22
BBBBATOM	3747	C	PHE	B	153	20.155	-48.075	-34.723	1.00	36.90
BBBBATOM	3748	O	PHE	B	153	20.407	-46.878	-34.879	1.00	37.54
BBBBATOM	3749	N	PRO	B	154	20.944	-49.040	-35.220	1.00	38.15
BBBBATOM	3750	CD	PRO	B	154	20.845	-50.482	-34.932	1.00	38.37
BBBBATOM	3751	CA	PRO	B	154	22.158	-48.751	-35.993	1.00	38.97
BBBBATOM	3752	CB	PRO	B	154	22.706	-50.143	-36.302	1.00	39.31
BBBBATOM	3753	CG	PRO	B	154	22.274	-50.941	-35.108	1.00	39.50
BBBBATOM	3754	C	PRO	B	154	21.964	-47.921	-37.266	1.00	39.90
BBBBATOM	3755	O	PRO	B	154	22.697	-46.958	-37.496	1.00	39.89
BBBBATOM	3756	N	ASN	B	155	20.979	-48.280	-38.088	1.00	40.46
BBBBATOM	3757	CA	ASN	B	155	20.765	-47.568	-39.346	1.00	41.08
BBBBATOM	3758	CB	ASN	B	155	21.135	-48.488	-40.510	1.00	43.63
BBBBATOM	3759	CG	ASN	B	155	22.618	-48.753	-40.585	1.00	45.00
BBBBATOM	3760	OD1	ASN	B	155	23.401	-47.861	-40.922	1.00	46.41
BBBBATOM	3761	ND2	ASN	B	155	23.019	-49.978	-40.259	1.00	45.20
BBBBATOM	3762	C	ASN	B	155	19.393	-46.966	-39.627	1.00	40.73
BBBBATOM	3763	O	ASN	B	155	19.145	-46.501	-40.742	1.00	41.01
BBBBATOM	3764	N	ALA	B	156	18.507	-46.956	-38.638	1.00	38.93
BBBBATOM	3765	CA	ALA	B	156	17.170	-46.407	-38.843	1.00	37.55
BBBBATOM	3766	CB	ALA	B	156	16.304	-46.689	-37.618	1.00	37.34
BBBBATOM	3767	C	ALA	B	156	17.209	-44.909	-39.123	1.00	36.36
BBBBATOM	3768	O	ALA	B	156	17.934	-44.171	-38.459	1.00	36.95
BBBBATOM	3769	N	GLU	B	157	16.428	-44.464	-40.107	1.00	35.76
BBBBATOM	3770	CA	GLU	B	157	16.367	-43.044	-40.460	1.00	34.40
BBBBATOM	3771	CB	GLU	B	157	15.375	-42.815	-41.613	1.00	34.84
BBBBATOM	3772	CG	GLU	B	157	15.246	-41.349	-42.055	1.00	34.91
BBBBATOM	3773	CD	GLU	B	157	14.171	-41.123	-43.117	1.00	36.66
BBBBATOM	3774	OE1	GLU	B	157	13.952	-39.951	-43.509	1.00	37.67
BBBBATOM	3775	OE2	GLU	B	157	13.543	-42.107	-43.563	1.00	35.62
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BBBBATOM	3777	O	GLU	B	157	14.941	-42.605	-38.574	1.00	33.04
BBBBATOM	3778	N	VAL	B	158	16.655	-41.185	-38.915	1.00	32.73
BBBBATOM	3779	CA	VAL	B	158	16.337	-40.344	-37.764	1.00	31.16
BBBBATOM	3780	CB	VAL	B	158	17.606	-39.680	-37.202	1.00	31.85
BBBBATOM	3781	CG1	VAL	B	158	17.238	-38.729	-36.073	1.00	31.22
BBBBATOM	3782	CG2	VAL	B	158	18.574	-40.752	-36.708	1.00	31.41
BBBBATOM	3783	C	VAL	B	158	15.352	-39.260	-38.178	1.00	30.27
BBBBATOM	3784	O	VAL	B	158	15.649	-38.445	-39.053	1.00	30.18
BBBBATOM	3785	N	VAL	B	159	14.186	-39.241	-37.544	1.00	28.57
BBBBATOM	3786	CA	VAL	B	159	13.155	-38.265	-37.889	1.00	28.10
BBBBATOM	3787	CB	VAL	B	159	11.942	-38.963	-38.535	1.00	27.81
BBBBATOM	3788	CG1	VAL	B	159	12.365	-39.667	-39.819	1.00	28.61

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BBBBATOM   3789  CG2 VAL B 159   11.336 -39.962 -37.548  1.00 27.61
BBBBATOM   3790  C   VAL B 159   12.636 -37.430 -36.725  1.00 27.64
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BBBBATOM   3792  N   GLY B 160   13.168 -37.662 -35.527  1.00 27.60
BBBBATOM   3793  CA  GLY B 160   12.724 -36.921 -34.355  1.00 26.93
BBBBATOM   3794  C   GLY B 160   11.331 -37.312 -33.883  1.00 26.66
BBBBATOM   3795  O   GLY B 160   10.757 -38.275 -34.384  1.00 26.71
BBBBATOM   3796  N   ASN B 161   10.797 -36.569 -32.914  1.00 25.68
BBBBATOM   3797  CA  ASN B 161    9.456 -36.807 -32.375  1.00 25.27
BBBBATOM   3798  CB  ASN B 161    9.481 -36.963 -30.849  1.00 23.89
BBBBATOM   3799  CG  ASN B 161   10.042 -38.285 -30.401  1.00 22.91
BBBBATOM   3800  OD1 ASN B 161    9.600 -39.335 -30.850  1.00 22.70
BBBBATOM   3801  ND2 ASN B 161   11.017 -38.243 -29.496  1.00 22.71
BBBBATOM   3802  C   ASN B 161    8.556 -35.61B -32.670  1.00 25.39
BBBBATOM   3803  O   ASN B 161    9.028 -34.499 -32.821  1.00 25.45
BBBBATOM   3804  N   PRO B 162    7.241 -35.849 -32.741  1.00 26.08
BBBBATOM   3805  CD  PRO B 162    6.533 -37.140 -32.710  1.00 25.20
BBBBATOM   3806  CA  PRO B 162    6.315 -34.747 -33.004  1.00 26.14
BBBBATOM   3807  CB  PRO B 162    4.952 -35.431 -32.976  1.00 25.76
BBBBATOM   3808  CG  PRO B 162    5.255 -36.821 -33.430  1.00 26.48
BBBBATOM   3809  C   PRO B 162    6.455 -33.728 -31.866  1.00 27.00
BBBBATOM   3810  O   PRO B 162    6.652 -34.102 -30.703  1.00 25.08
BBBBATOM   3811  N   VAL B 163    6.355 -32.446 -32.203  1.00 27.54
BBBBATOM   3812  CA  VAL B 163    6.456 -31.379 -31.216  1.00 27.75
BBBBATOM   3813  CB  VAL B 163    7.748 -30.561 -31.421  1.00 28.81
BBBBATOM   3814  CG1 VAL B 163    7.839 -29.451 -30.381  1.00 28.20
BBBBATOM   3815  CG2 VAL B 163    8.958 -31.471 -31.335  1.00 27.87
BBBBATOM   3816  C   VAL B 163    5.261 -30.440 -31.365  1.00 29.43
BBBBATOM   3817  O   VAL B 163    4.777 -30.227 -32.476  1.00 28.49
BBBBATOM   3818  N   ARG B 164    4.790 -29.891 -30.246  1.00 29.93
BBBBATOM   3819  CA  ARG B 164    3.667 -28.953 -30.246  1.00 32.36
BBBBATOM   3820  CB  ARG B 164    3.430 -28.411 -28.833  1.00 34.56
BBBBATOM   3821  CG  ARG B 164    2.967 -29.439 -27.832  1.00 38.34
BBBBATOM   3822  CD  ARG B 164    3.067 -28.889 -26.417  1.00 41.59
BBBBATOM   3823  NE  ARG B 164    2.481 -27.555 -26.299  1.00 44.08
BBBBATOM   3824  CZ  ARG B 164    2.307 -26.919 -25.144  1.00 45.79
BBBBATOM   3825  NH1 ARG B 164    2.673 -27.499 -24.008  1.00 46.89
BBBBATOM   3826  NH2 ARG B 164    1.769 -25.705 -25.123  1.00 47.50
BBBBATOM   3827  C   ARG B 164    3.939 -27.775 -31.187  1.00 31.56
BBBBATOM   3828  O   ARG B 164    5.031 -27.212 -31.191  1.00 30.03
BBBBATOM   3829  N   THR B 165    2.928 -27.401 -31.965  1.00 32.06
BBBBATOM   3830  CA  THR B 165    3.038 -26.307 -32.924  1.00 31.74
BBBBATOM   3831  CB  THR B 165    1.701 -26.104 -33.678  1.00 32.51
BBBBATOM   3832  OG1 THR B 165    1.198 -27.375 -34.094  1.00 32.54
BBBBATOM   3833  CG2 THR B 165    1.907 -25.239 -34.916  1.00 32.14
BBBBATOM   3834  C   THR B 165    3.445 -24.976 -32.295  1.00 31.49
BBBBATOM   3835  O   THR B 165    4.236 -24.238 -32.872  1.00 31.48
BBBBATOM   3836  N   ASP B 166    2.907 -24.664 -31.120  1.00 30.86
BBBBATOM   3837  CA  ASP B 166    3.252 -23.404 -30.466  1.00 30.64
BBBBATOM   3838  CB  ASP B 166    2.358 -23.163 -29.242  1.00 33.08
BBBBATOM   3839  CG  ASP B 166    2.185 -24.400 -28.384  1.00 35.24
BBBBATOM   3840  OD1 ASP B 166    1.315 -24.373 -27.485  1.00 38.19
BBBBATOM   3841  OD2 ASP B 166    2.908 -25.393 -28.603  1.00 37.17
BBBBATOM   3842  C   ASP B 166    4.729 -23.338 -30.084  1.00 28.64
BBBBATOM   3843  O   ASP B 166    5.321 -22.259 -30.076  1.00 27.92
BBBBATOM   3844  N   VAL B 167    5.328 -24.485 -29.773  1.00 27.08
BBBBATOM   3845  CA  VAL B 167    6.746 -24.503 -29.440  1.00 25.91
BBBBATOM   3846  CB  VAL B 167    7.171 -25.824 -28.757  1.00 25.96
BBBBATOM   3847  CG1 VAL B 167    8.687 -25.844 -28.586  1.00 24.67
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BBBBATOM   3849  C   VAL B 167    7.548 -24.361 -30.736  1.00 25.54
BBBBATOM   3850  O   VAL B 167    8.548 -23.642 -30.787  1.00 25.58
BBBBATOM   3851  N   LEU B 168    7.108 -25.059 -31.778  1.00 26.75
BBBBATOM   3852  CA  LEU B 168    7.780 -25.002 -33.075  1.00 28.46
BBBBATOM   3853  CB  LEU B 168    7.085 -25.930 -34.080  1.00 28.40
BBBBATOM   3854  CG  LEU B 168    7.205 -27.440 -33.890  1.00 28.67
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BBBBATOM	3855	CD1	LEU	B	168	6.254	-28.161	-34.854	1.00	30.19
BBBBATOM	3856	CD2	LEU	B	168	8.647	-27.668	-34.129	1.00	28.82
BBBBATOM	3857	C	LEU	B	168	7.766	-23.584	-33.632	1.00	29.14
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BBBBATOM	3859	N	ALA	B	169	6.741	-22.823	-33.267	1.00	30.35
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BBBBATOM	3872	N	PRO	B	171	10.525	-18.099	-31.897	1.00	29.71
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BBBBATOM	3875	CB	PRO	B	171	11.665	-16.054	-32.033	1.00	29.54
BBBBATOM	3876	CG	PRO	B	171	10.261	-15.810	-31.605	1.00	30.96
BBBBATOM	3877	C	PRO	B	171	12.900	-18.226	-32.374	1.00	30.39
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BBBBATOM	3879	N	LEU	B	172	13.883	-18.097	-33.263	1.00	28.62
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BBBBATOM	3881	CB	LEU	B	172	16.106	-18.557	-34.247	1.00	29.88
BBBBATOM	3882	CG	LEU	B	172	15.800	-19.149	-35.628	1.00	32.18
BBBBATOM	3883	CD1	LEU	B	172	15.593	-20.656	-35.510	1.00	32.75
BBBBATOM	3884	CD2	LEU	B	172	14.573	-18.476	-36.222	1.00	33.92
BBBBATOM	3885	C	LEU	B	172	15.805	-18.206	-31.805	1.00	26.61
BBBBATOM	3886	O	LEU	B	172	15.478	-17.093	-31.388	1.00	26.45
BBBBATOM	3887	N	PRO	B	173	16.735	-18.959	-31.190	1.00	25.73
BBBBATOM	3888	CD	PRO	B	173	17.093	-20.345	-31.550	1.00	24.63
BBBBATOM	3889	CA	PRO	B	173	17.450	-18.550	-29.977	1.00	25.25
BBBBATOM	3890	CB	PRO	B	173	18.512	-19.635	-29.827	1.00	25.04
BBBBATOM	3891	CG	PRO	B	173	17.818	-20.831	-30.309	1.00	24.90
BBBBATOM	3892	C	PRO	B	173	18.066	-17.145	-29.999	1.00	24.24
BBBBATOM	3893	O	PRO	B	173	17.791	-16.337	-29.116	1.00	22.89
BBBBATOM	3894	N	GLN	B	174	18.899	-16.850	-30.995	1.00	24.48
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BBBBATOM	3896	CB	GLN	B	174	20.384	-15.382	-32.313	1.00	26.10
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BBBBATOM	3908	OE1	GLN	B	175	12.247	-12.422	-34.215	1.00	38.98
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BBBBATOM	3919	NH1	ARG	B	176	15.121	-19.233	-26.107	1.00	41.22
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BBBBATOM   3922  O   ARG B 176   14.933 -13.414 -26.467  1.00 26.70
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BBBBATOM   3972  CA  VAL B 184   19.524 -16.146 -15.729  1.00 18.01
BBBBATOM   3973  CB  VAL B 184   20.597 -17.248 -15.549  1.00 17.45
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BBBBATOM   3985  NH1 ARG B 185   12.977 -13.197 -20.391  1.00 19.85
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BBBBATOM  4091  NE2 GLN B 200      13.155 -34.502  -2.151  1.00 37.28
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BBBBATOM  4103  CB  MET B 202      14.558 -25.827  -7.397  1.00 22.29
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BBBBATOM  4107  C   MET B 202      15.489 -24.926  -5.229  1.00 23.47
BBBBATOM  4108  O   MET B 202      16.189 -23.929  -5.354  1.00 24.40
BBBBATOM  4109  N   PRO B 203      14.636 -25.059  -4.192  1.00 24.12
BBBBATOM  4110  CD  PRO B 203      13.518 -25.991  -3.970  1.00 22.27
BBBBATOM  4111  CA  PRO B 203      14.608 -23.963  -3.220  1.00 23.84
BBBBATOM  4112  CB  PRO B 203      13.553 -24.424  -2.217  1.00 24.46
BBBBATOM  4113  CG  PRO B 203      12.593 -25.178  -3.084  1.00 24.04
BBBBATOM  4114  C   PRO B 203      15.987 -23.731  -2.573  1.00 24.07
BBBBATOM  4115  O   PRO B 203      16.395 -22.593  -2.343  1.00 23.18
BBBBATOM  4116  N   GLN B 204      16.706 -24.814  -2.290  1.00 25.26
BBBBATOM  4117  CA  GLN B 204      18.033 -24.708  -1.684  1.00 26.34
BBBBATOM  4118  CB  GLN B 204      18.474 -26.078  -1.157  1.00 28.67
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BBBBATOM	4119	CG	GLN	B	204	17.555	-26.626	-0.065	1.00	33.65
BBBBATOM	4120	CD	GLN	B	204	17.885	-28.059	0.328	1.00	37.09
BBBBATOM	4121	OE1	GLN	B	204	18.991	-28.354	0.792	1.00	39.30
BBBBATOM	4122	NE2	GLN	B	204	16.924	-28.960	0.140	1.00	38.32
BBBBATOM	4123	C	GLN	B	204	19.030	-24.177	-2.717	1.00	25.36
BBBBATOM	4124	O	GLN	B	204	19.985	-23.466	-2.385	1.00	24.98
BBBBATOM	4125	N	VAL	B	205	18.806	-24.522	-3.978	1.00	24.46
BBBBATOM	4126	CA	VAL	B	205	19.672	-24.033	-5.043	1.00	24.44
BBBBATOM	4127	CB	VAL	B	205	19.288	-24.634	-6.409	1.00	24.84
BBBBATOM	4128	CG1	VAL	B	205	20.039	-23.906	-7.534	1.00	23.72
BBBBATOM	4129	CG2	VAL	B	205	19.614	-26.110	-6.428	1.00	22.91
BBBBATOM	4130	C	VAL	B	205	19.511	-22.515	-5.110	1.00	23.79
BBBBATOM	4131	O	VAL	B	205	20.487	-21.789	-5.270	1.00	25.25
BBBBATOM	4132	N	ALA	B	206	18.273	-22.044	-4.972	1.00	24.12
BBBBATOM	4133	CA	ALA	B	206	17.980	-20.610	-5.013	1.00	22.84
BBBBATOM	4134	CB	ALA	B	206	16.466	-20.377	-4.908	1.00	21.55
BBBBATOM	4135	C	ALA	B	206	18.700	-19.862	-3.890	1.00	24.09
BBBBATOM	4136	O	ALA	B	206	19.174	-18.740	-4.081	1.00	24.90
BBBBATOM	4137	N	ALA	B	207	18.768	-20.477	-2.713	1.00	25.15
BBBBATOM	4138	CA	ALA	B	207	19.442	-19.857	-1.576	1.00	26.65
BBBBATOM	4139	CB	ALA	B	207	19.260	-20.710	-0.324	1.00	27.83
BBBBATOM	4140	C	ALA	B	207	20.924	-19.686	-1.879	1.00	26.96
BBBBATOM	4141	O	ALA	B	207	21.537	-18.693	-1.493	1.00	27.82
BBBBATOM	4142	N	LYS	B	208	21.498	-20.651	-2.586	1.00	27.19
BBBBATOM	4143	CA	LYS	B	208	22.915	-20.595	-2.919	1.00	28.31
BBBBATOM	4144	CB	LYS	B	208	23.432	-21.989	-3.300	1.00	29.85
BBBBATOM	4145	CG	LYS	B	208	23.030	-23.088	-2.329	1.00	32.97
BBBBATOM	4146	CD	LYS	B	208	23.264	-22.667	-0.886	1.00	35.74
BBBBATOM	4147	CE	LYS	B	208	22.689	-23.689	0.084	1.00	37.28
BBBBATOM	4148	NZ	LYS	B	208	21.227	-23.899	-0.135	1.00	35.29
BBBBATOM	4149	C	LYS	B	208	23.237	-19.624	-4.050	1.00	27.83
BBBBATOM	4150	O	LYS	B	208	24.286	-18.978	-4.033	1.00	27.46
BBBBATOM	4151	N	LEU	B	209	22.341	-19.517	-5.028	1.00	26.04
BBBBATOM	4152	CA	LEU	B	209	22.577	-18.640	-6.171	1.00	25.68
BBBBATOM	4153	CB	LEU	B	209	21.975	-19.268	-7.435	1.00	25.08
BBBBATOM	4154	CG	LEU	B	209	22.534	-20.638	-7.844	1.00	25.01
BBBBATOM	4155	CD1	LEU	B	209	21.797	-21.151	-9.074	1.00	25.67
BBBBATOM	4156	CD2	LEU	B	209	24.029	-20.528	-8.119	1.00	25.13
BBBBATOM	4157	C	LEU	B	209	22.075	-17.200	-6.007	1.00	25.59
BBBBATOM	4158	O	LEU	B	209	22.496	-16.313	-6.742	1.00	25.26
BBBBATOM	4159	N	GLY	B	210	21.185	-16.970	-5.045	1.00	26.27
BBBBATOM	4160	CA	GLY	B	210	20.675	-15.628	-4.804	1.00	26.56
BBBBATOM	4161	C	GLY	B	210	20.238	-14.836	-6.030	1.00	27.75
BBBBATOM	4162	O	GLY	B	210	19.518	-15.349	-6.889	1.00	27.68
BBBBATOM	4163	N	ASP	B	211	20.696	-13.585	-6.105	1.00	27.93
BBBBATOM	4164	CA	ASP	B	211	20.370	-12.647	-7.190	1.00	28.28
BBBBATOM	4165	CB	ASP	B	211	21.011	-11.283	-6.906	1.00	29.89
BBBBATOM	4166	CG	ASP	B	211	20.351	-10.545	-5.768	1.00	31.43
BBBBATOM	4167	OD1	ASP	B	211	20.864	-9.469	-5.398	1.00	32.43
BBBBATOM	4168	OD2	ASP	B	211	19.323	-11.025	-5.249	1.00	33.41
BBBBATOM	4169	C	ASP	B	211	20.768	-13.035	-8.615	1.00	27.77
BBBBATOM	4170	O	ASP	B	211	20.320	-12.397	-9.578	1.00	26.32
BBBBATOM	4171	N	SER	B	212	21.616	-14.048	-8.753	1.00	25.75
BBBBATOM	4172	CA	SER	B	212	22.098	-14.474	-10.067	1.00	25.73
BBBBATOM	4173	CB	SER	B	212	23.331	-15.376	-9.904	1.00	26.63
BBBBATOM	4174	OG	SER	B	212	22.971	-16.596	-9.282	1.00	26.71
BBBBATOM	4175	C	SER	B	212	21.062	-15.185	-10.943	1.00	23.61
BBBBATOM	4176	O	SER	B	212	21.262	-15.334	-12.147	1.00	22.28
BBBBATOM	4177	N	VAL	B	213	19.969	-15.644	-10.344	1.00	23.16
BBBBATOM	4178	CA	VAL	B	213	18.925	-16.308	-11.116	1.00	20.76
BBBBATOM	4179	CB	VAL	B	213	18.952	-17.867	-10.989	1.00	21.69
BBBBATOM	4180	CG1	VAL	B	213	20.318	-18.423	-11.375	1.00	19.84
BBBBATOM	4181	CG2	VAL	B	213	18.564	-18.288	-9.576	1.00	20.36
BBBBATOM	4182	C	VAL	B	213	17.535	-15.871	-10.677	1.00	21.41
BBBBATOM	4183	O	VAL	B	213	17.328	-15.396	-9.554	1.00	20.58
BBBBATOM	4184	N	THR	B	214	16.593	-16.021	-11.595	1.00	19.82

BBBBATOM	4185	CA	THR	B	214	15.204	-15.726	-11.337	1.00	19.60
BBBBATOM	4186	CB	THR	B	214	14.718	-14.278	-12.126	1.00	21.35
BBBBATOM	4187	OG1	THR	B	214	13.323	-14.273	-11.870	1.00	21.93
BBBBATOM	4188	CG2	THR	B	214	14.983	-14.633	-13.622	1.00	19.52
BBBBATOM	4189	C	THR	B	214	14.543	-17.021	-11.791	1.00	20.24
BBBBATOM	4190	O	THR	B	214	14.803	-17.533	-12.893	1.00	18.70
BBBBATOM	4191	N	ILE	B	215	13.706	-17.569	-10.921	1.00	19.21
BBBBATOM	4192	CA	ILE	B	215	13.076	-18.850	-11.169	1.00	18.75
BBBBATOM	4193	CB	ILE	B	215	13.417	-19.828	-10.008	1.00	18.82
BBBBATOM	4194	CG2	ILE	B	215	12.690	-21.157	-10.194	1.00	19.53
BBBBATOM	4195	CG1	ILE	B	215	14.934	-20.030	-9.931	1.00	19.76
BBBBATOM	4196	CD1	ILE	B	215	15.421	-20.656	-8.600	1.00	19.40
BBBBATOM	4197	C	ILE	B	215	11.568	-18.837	-11.315	1.00	19.26
BBBBATOM	4198	O	ILE	B	215	10.874	-18.025	-10.699	1.00	18.28
BBBBATOM	4199	N	TRP	B	216	11.089	-19.737	-12.167	1.00	18.93
BBBBATOM	4200	CA	TRP	B	216	9.661	-19.973	-12.378	1.00	19.34
BBBBATOM	4201	CB	TRP	B	216	9.222	-19.631	-13.797	1.00	18.97
BBBBATOM	4202	CG	TRP	B	216	7.757	-19.897	-14.065	1.00	20.09
BBBBATOM	4203	CD2	TRP	B	216	7.015	-19.467	-15.211	1.00	19.61
BBBBATOM	4204	CE2	TRP	B	216	5.705	-19.988	-15.085	1.00	19.98
BBBBATOM	4205	CE3	TRP	B	216	7.329	-18.690	-16.333	1.00	19.39
BBBBATOM	4206	CD1	TRP	B	216	6.888	-20.639	-13.303	1.00	19.30
BBBBATOM	4207	NE1	TRP	B	216	5.653	-20.700	-13.914	1.00	20.95
BBBBATOM	4208	CZ2	TRP	B	216	4.713	-19.759	-16.043	1.00	22.06
BBBBATOM	4209	CZ3	TRP	B	216	6.336	-18.459	-17.288	1.00	20.42
BBBBATOM	4210	CH2	TRP	B	216	5.047	-18.993	-17.134	1.00	21.16
BBBBATOM	4211	C	TRP	B	216	9.629	-21.479	-12.176	1.00	19.95
BBBBATOM	4212	O	TRP	B	216	10.114	-22.241	-13.010	1.00	19.91
BBBBATOM	4213	N	HIS	B	217	9.067	-21.897	-11.050	1.00	21.62
BBBBATOM	4214	CA	HIS	B	217	9.015	-23.303	-10.680	1.00	21.06
BBBBATOM	4215	CB	HIS	B	217	9.553	-23.419	-9.242	1.00	20.56
BBBBATOM	4216	CG	HIS	B	217	9.717	-24.824	-8.747	1.00	21.95
BBBBATOM	4217	CD2	HIS	B	217	8.915	-25.910	-8.846	1.00	22.12
BBBBATOM	4218	ND1	HIS	B	217	10.807	-25.219	-8.002	1.00	23.39
BBBBATOM	4219	CE1	HIS	B	217	10.670	-26.490	-7.663	1.00	21.82
BBBBATOM	4220	NE2	HIS	B	217	9.530	-26.933	-8.162	1.00	22.14
BBBBATOM	4221	C	HIS	B	217	7.596	-23.870	-10.795	1.00	21.27
BBBBATOM	4222	O	HIS	B	217	6.655	-23.334	-10.214	1.00	21.69
BBBBATOM	4223	N	GLN	B	218	7.448	-24.940	-11.567	1.00	20.83
BBBBATOM	4224	CA	GLN	B	218	6.149	-25.594	-11.735	1.00	24.30
BBBBATOM	4225	CB	GLN	B	218	5.915	-25.935	-13.206	1.00	23.84
BBBBATOM	4226	CG	GLN	B	218	4.561	-26.558	-13.495	1.00	25.91
BBBBATOM	4227	CD	GLN	B	218	4.637	-28.060	-13.673	1.00	26.52
BBBBATOM	4228	OE1	GLN	B	218	3.757	-28.793	-13.214	1.00	28.05
BBBBATOM	4229	NE2	GLN	B	218	5.680	-28.529	-14.360	1.00	25.20
BBBBATOM	4230	C	GLN	B	218	6.173	-26.854	-10.854	1.00	24.64
BBBBATOM	4231	O	GLN	B	218	6.780	-27.866	-11.199	1.00	25.73
BBBBATOM	4232	N	SER	B	219	5.502	-26.756	-9.709	1.00	26.38
BBBBATOM	4233	CA	SER	B	219	5.463	-27.800	-8.684	1.00	26.73
BBBBATOM	4234	CB	SER	B	219	4.947	-27.188	-7.380	1.00	28.26
BBBBATOM	4235	OG	SER	B	219	3.563	-26.881	-7.488	1.00	26.22
BBBBATOM	4236	C	SER	B	219	4.689	-29.096	-8.914	1.00	27.58
BBBBATOM	4237	O	SER	B	219	5.014	-30.122	-8.320	1.00	26.39
BBBBATOM	4238	N	GLY	B	220	3.662	-29.054	-9.750	1.00	28.58
BBBBATOM	4239	CA	GLY	B	220	2.855	-30.242	-9.961	1.00	30.53
BBBBATOM	4240	C	GLY	B	220	1.596	-30.110	-9.111	1.00	31.96
BBBBATOM	4241	O	GLY	B	220	1.523	-29.248	-8.233	1.00	30.92
BBBBATOM	4242	N	LYS	B	221	0.608	-30.965	-9.358	1.00	33.93
BBBBATOM	4243	CA	LYS	B	221	-0.657	-30.914	-8.628	1.00	35.12
BBBBATOM	4244	CB	LYS	B	221	-1.573	-32.049	-9.094	1.00	37.88
BBBBATOM	4245	CG	LYS	B	221	-2.942	-32.055	-8.427	1.00	40.51
BBBBATOM	4246	CD	LYS	B	221	-3.792	-33.215	-8.934	1.00	42.62
BBBBATOM	4247	CE	LYS	B	221	-5.162	-33.249	-8.260	1.00	43.67
BBBBATOM	4248	NZ	LYS	B	221	-6.002	-34.383	-8.763	1.00	45.38
BBBBATOM	4249	C	LYS	B	221	-0.545	-30.950	-7.103	1.00	35.13
BBBBATOM	4250	O	LYS	B	221	0.110	-31.823	-6.531	1.00	34.60

BBBBATOM	4251	N	GLY	B	222	-1.187	-29.979	-6.461	1.00	34.79
BBBBATOM	4252	CA	GLY	B	222	-1.195	-29.899	-5.011	1.00	35.34
BBBBATOM	4253	C	GLY	B	222	0.111	-29.594	-4.299	1.00	35.61
BBBBATOM	4254	O	GLY	B	222	0.163	-29.678	-3.071	1.00	35.51
BBBBATOM	4255	N	SER	B	223	1.158	-29.234	-5.038	1.00	34.65
BBBBATOM	4256	CA	SER	B	223	2.451	-28.934	-4.418	1.00	33.98
BBBBATOM	4257	CB	SER	B	223	3.552	-29.781	-5.062	1.00	35.02
BBBBATOM	4258	OG	SER	B	223	3.303	-31.168	-4.897	1.00	36.07
BBBBATOM	4259	C	SER	B	223	2.839	-27.454	-4.504	1.00	33.55
BBBBATOM	4260	O	SER	B	223	3.930	-27.063	-4.086	1.00	31.72
BBBBATOM	4261	N	GLN	B	224	1.941	-26.639	-5.044	1.00	33.22
BBBBATOM	4262	CA	GLN	B	224	2.187	-25.208	-5.186	1.00	33.71
BBBBATOM	4263	CB	GLN	B	224	0.954	-24.539	-5.799	1.00	35.45
BBBBATOM	4264	CG	GLN	B	224	1.160	-23.120	-6.337	1.00	37.82
BBBBATOM	4265	CD	GLN	B	224	1.344	-22.076	-5.249	1.00	40.08
BBBBATOM	4266	OE1	GLN	B	224	0.669	-22.111	-4.217	1.00	40.97
BBBBATOM	4267	NE2	GLN	B	224	2.244	-21.124	-5.486	1.00	40.08
BBBBATOM	4268	C	GLN	B	224	2.510	-24.560	-3.840	1.00	33.86
BBBBATOM	4269	O	GLN	B	224	3.512	-23.856	-3.697	1.00	33.38
BBBBATOM	4270	N	GLN	B	225	1.659	-24.814	-2.850	1.00	33.06
BBBBATOM	4271	CA	GLN	B	225	1.823	-24.239	-1.519	1.00	32.32
BBBBATOM	4272	CB	GLN	B	225	0.624	-24.619	-0.640	1.00	35.12
BBBBATOM	4273	CG	GLN	B	225	-0.743	-24.143	-1.151	1.00	36.85
BBBBATOM	4274	CD	GLN	B	225	-1.144	-24.751	-2.495	1.00	39.09
BBBBATOM	4275	OE1	GLN	B	225	-0.914	-25.937	-2.759	1.00	39.42
BBBBATOM	4276	NE2	GLN	B	225	-1.768	-23.937	-3.345	1.00	40.13
BBBBATOM	4277	C	GLN	B	225	3.117	-24.606	-0.788	1.00	30.73
BBBBATOM	4278	O	GLN	B	225	3.766	-23.742	-0.202	1.00	30.36
BBBBATOM	4279	N	SER	B	226	3.494	-25.878	-0.817	1.00	29.26
BBBBATOM	4280	CA	SER	B	226	4.701	-26.309	-0.122	1.00	28.30
BBBBATOM	4281	CB	SER	B	226	4.727	-27.834	0.003	1.00	29.10
BBBBATOM	4282	OG	SER	B	226	4.563	-28.461	-1.254	1.00	32.61
BBBBATOM	4283	C	SER	B	226	5.991	-25.809	-0.771	1.00	26.41
BBBBATOM	4284	O	SER	B	226	6.950	-25.486	-0.073	1.00	25.24
BBBBATOM	4285	N	VAL	B	227	6.019	-25.738	-2.099	1.00	25.21
BBBBATOM	4286	CA	VAL	B	227	7.214	-25.247	-2.791	1.00	24.28
BBBBATOM	4287	CB	VAL	B	227	7.150	-25.527	-4.317	1.00	23.32
BBBBATOM	4288	CG1	VAL	B	227	8.368	-24.914	-5.028	1.00	20.67
BBBBATOM	4289	CG2	VAL	B	227	7.117	-27.024	-4.563	1.00	22.45
BBBBATOM	4290	C	VAL	B	227	7.335	-23.743	-2.545	1.00	24.34
BBBBATOM	4291	O	VAL	B	227	8.421	-23.240	-2.281	1.00	25.50
BBBBATOM	4292	N	GLU	B	228	6.209	-23.035	-2.623	1.00	26.12
BBBBATOM	4293	CA	GLU	B	228	6.178	-21.592	-2.387	1.00	27.23
BBBBATOM	4294	CB	GLU	B	228	4.735	-21.075	-2.476	1.00	28.60
BBBBATOM	4295	CG	GLU	B	228	4.558	-19.586	-2.184	1.00	30.24
BBBBATOM	4296	CD	GLU	B	228	4.938	-18.688	-3.356	1.00	31.99
BBBBATOM	4297	OE1	GLU	B	228	5.012	-17.452	-3.159	1.00	31.68
BBBBATOM	4298	OE2	GLU	B	228	5.154	-19.212	-4.471	1.00	32.04
BBBBATOM	4299	C	GLU	B	228	6.746	-21.327	-0.994	1.00	27.95
BBBBATOM	4300	O	GLU	B	228	7.511	-20.383	-0.787	1.00	27.32
BBBBATOM	4301	N	GLN	B	229	6.374	-22.178	-0.041	1.00	28.66
BBBBATOM	4302	CA	GLN	B	229	6.853	-22.046	1.329	1.00	28.38
BBBBATOM	4303	CB	GLN	B	229	6.082	-22.990	2.261	1.00	31.03
BBBBATOM	4304	CG	GLN	B	229	6.570	-22.946	3.700	1.00	35.48
BBBBATOM	4305	CD	GLN	B	229	5.780	-23.860	4.615	1.00	38.01
BBBBATOM	4306	OE1	GLN	B	229	4.548	-23.810	4.645	1.00	39.26
BBBBATOM	4307	NE2	GLN	B	229	6.484	-24.697	5.370	1.00	38.61
BBBBATOM	4308	C	GLN	B	229	8.338	-22.362	1.407	1.00	27.09
BBBBATOM	4309	O	GLN	B	229	9.084	-21.697	2.124	1.00	28.29
BBBBATOM	4310	N	ALA	B	230	8.771	-23.385	0.677	1.00	26.97
BBBBATOM	4311	CA	ALA	B	230	10.185	-23.754	0.682	1.00	26.18
BBBBATOM	4312	CB	ALA	B	230	10.412	-24.984	-0.184	1.00	25.07
BBBBATOM	4313	C	ALA	B	230	11.054	-22.588	0.192	1.00	26.36
BBBBATOM	4314	O	ALA	B	230	12.119	-22.317	0.755	1.00	25.04
BBBBATOM	4315	N	TYR	B	231	10.605	-21.895	-0.854	1.00	25.85
BBBBATOM	4316	CA	TYR	B	231	11.371	-20.766	-1.366	1.00	25.47

BBBBATOM	4317	CB	TYR	B	231	10.762	-20.248	-2.678	1.00 24.72
BBBBATOM	4318	CG	TYR	B	231	11.236	-21.014	-3.905	1.00 23.66
BBBBATOM	4319	CD1	TYR	B	231	12.546	-20.869	-4.381	1.00 23.97
BBBBATOM	4320	CE1	TYR	B	231	13.006	-21.599	-5.488	1.00 21.40
BBBBATOM	4321	CD2	TYR	B	231	10.393	-21.905	-4.567	1.00 22.63
BBBBATOM	4322	CE2	TYR	B	231	10.841	-22.641	-5.681	1.00 22.71
BBBBATOM	4323	CZ	TYR	B	231	12.151	-22.480	-6.128	1.00 21.91
BBBBATOM	4324	OH	TYR	B	231	12.600	-23.214	-7.199	1.00 21.69
BBBBATOM	4325	C	TYR	B	231	11.450	-19.639	-0.336	1.00 26.53
BBBBATOM	4326	O	TYR	B	231	12.498	-19.011	-0.175	1.00 26.32
BBBBATOM	4327	N	ALA	B	232	10.345	-19.380	0.361	1.00 26.28
BBBBATOM	4328	CA	ALA	B	232	10.342	-18.322	1.368	1.00 27.51
BBBBATOM	4329	CB	ALA	B	232	8.930	-18.109	1.910	1.00 28.09
BBBBATOM	4330	C	ALA	B	232	11.303	-18.695	2.499	1.00 28.03
BBBBATOM	4331	O	ALA	B	232	12.069	-17.858	2.983	1.00 27.93
BBBBATOM	4332	N	GLU	B	233	11.263	-19.958	2.911	1.00 29.43
BBBBATOM	4333	CA	GLU	B	233	12.145	-20.441	3.966	1.00 30.87
BBBBATOM	4334	CB	GLU	B	233	11.772	-21.877	4.344	1.00 33.60
BBBBATOM	4335	CG	GLU	B	233	10.491	-21.973	5.170	1.00 37.67
BBBBATOM	4336	CD	GLU	B	233	10.077	-23.404	5.461	1.00 40.35
BBBBATOM	4337	OE1	GLU	B	233	10.964	-24.283	5.525	1.00 42.97
BBBBATOM	4338	OE2	GLU	B	233	8.864	-23.649	5.641	1.00 41.95
BBBBATOM	4339	C	GLU	B	233	13.606	-20.369	3.530	1.00 30.58
BBBBATOM	4340	O	GLU	B	233	14.499	-20.202	4.359	1.00 30.82
BBBBATOM	4341	N	ALA	B	234	13.850	-20.485	2.227	1.00 29.17
BBBBATOM	4342	CA	ALA	B	234	15.215	-20.417	1.714	1.00 28.48
BBBBATOM	4343	CB	ALA	B	234	15.310	-21.110	0.354	1.00 27.71
BBBBATOM	4344	C	ALA	B	234	15.649	-18.961	1.588	1.00 27.73
BBBBATOM	4345	O	ALA	B	234	16.787	-18.677	1.213	1.00 27.34
BBBBATOM	4346	N	GLY	B	235	14.731	-18.045	1.890	1.00 26.74
BBBBATOM	4347	CA	GLY	B	235	15.033	-16.627	1.815	1.00 26.23
BBBBATOM	4348	C	GLY	B	235	14.946	-16.009	0.426	1.00 26.13
BBBBATOM	4349	O	GLY	B	235	15.483	-14.924	0.198	1.00 25.67
BBBBATOM	4350	N	GLN	B	236	14.284	-16.696	-0.502	1.00 25.36
BBBBATOM	4351	CA	GLN	B	236	14.121	-16.198	-1.870	1.00 25.53
BBBBATOM	4352	CB	GLN	B	236	14.940	-17.043	-2.852	1.00 25.84
BBBBATOM	4353	CG	GLN	B	236	16.436	-17.074	-2.603	1.00 27.18
BBBBATOM	4354	CD	GLN	B	236	17.080	-15.705	-2.661	1.00 28.96
BBBBATOM	4355	OE1	GLN	B	236	16.686	-14.850	-3.456	1.00 30.03
BBBBATOM	4356	NE2	GLN	B	236	18.092	-15.495	-1.829	1.00 29.39
BBBBATOM	4357	C	GLN	B	236	12.641	-16.298	-2.232	1.00 24.12
BBBBATOM	4358	O	GLN	B	236	12.262	-17.002	-3.167	1.00 23.31
BBBBATOM	4359	N	PRO	B	237	11.783	-15.578	-1.497	1.00 24.40
BBBBATOM	4360	CD	PRO	B	237	12.143	-14.580	-0.473	1.00 24.52
BBBBATOM	4361	CA	PRO	B	237	10.336	-15.587	-1.720	1.00 24.65
BBBBATOM	4362	CB	PRO	B	237	9.808	-14.798	-0.527	1.00 25.37
BBBBATOM	4363	CG	PRO	B	237	10.862	-13.773	-0.340	1.00 25.24
BBBBATOM	4364	C	PRO	B	237	9.837	-15.012	-3.043	1.00 25.33
BBBBATOM	4365	O	PRO	B	237	8.720	-15.313	-3.465	1.00 24.93
BBBBATOM	4366	N	GLN	B	238	10.663	-14.197	-3.690	1.00 24.47
BBBBATOM	4367	CA	GLN	B	238	10.277	-13.558	-4.945	1.00 24.29
BBBBATOM	4368	CB	GLN	B	238	11.281	-12.455	-5.306	1.00 23.76
BBBBATOM	4369	CG	GLN	B	238	12.622	-12.945	-5.852	1.00 25.22
BBBBATOM	4370	CD	GLN	B	238	13.535	-13.523	-4.783	1.00 26.90
BBBBATOM	4371	OE1	GLN	B	238	13.188	-13.550	-3.600	1.00 28.05
BBBBATOM	4372	NE2	GLN	B	238	14.712	-13.983	-5.195	1.00 25.61
BBBBATOM	4373	C	GLN	B	238	10.108	-14.489	-6.143	1.00 23.41
BBBBATOM	4374	O	GLN	B	238	9.485	-14.112	-7.139	1.00 20.49
BBBBATOM	4375	N	HIS	B	239	10.655	-15.700	-6.069	1.00 22.66
BBBBATOM	4376	CA	HIS	B	239	10.526	-16.608	-7.201	1.00 22.08
BBBBATOM	4377	CB	HIS	B	239	11.432	-17.829	-7.008	1.00 22.41
BBBBATOM	4378	CG	HIS	B	239	12.891	-17.488	-6.998	1.00 20.93
BBBBATOM	4379	CD2	HIS	B	239	13.869	-17.774	-6.104	1.00 20.09
BBBBATOM	4380	ND1	HIS	B	239	13.488	-16.743	-7.992	1.00 20.30
BBBBATOM	4381	CE1	HIS	B	239	14.769	-16.582	-7.711	1.00 22.38
BBBBATOM	4382	NE2	HIS	B	239	15.025	-17.197	-6.569	1.00 19.62

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BBBBATOM   4383  C   HIS B 239      9.076 -17.024  -7.433  1.00 22.98
BBBBATOM   4384  O   HIS B 239      8.293 -17.161  -6.490  1.00 21.86
BBBBATOM   4385  N   LYS B 240      8.727 -17.209  -8.703  1.00 21.76
BBBBATOM   4386  CA  LYS B 240      7.375 -17.589  -9.105  1.00 23.26
BBBBATOM   4387  CB  LYS B 240      7.112 -17.102 -10.534  1.00 23.38
BBBBATOM   4388  CG  LYS B 240      5.718 -17.385 -11.079  1.00 24.06
BBBBATOM   4389  CD  LYS B 240      5.701 -17.155 -12.585  1.00 23.93
BBBBATOM   4390  CE  LYS B 240      4.315 -17.309 -13.193  1.00 23.72
BBBBATOM   4391  NZ  LYS B 240      3.478 -16.129 -12.884  1.00 21.82
BBBBATOM   4392  C   LYS B 240      7.149 -19.091  -9.046  1.00 23.38
BBBBATOM   4393  O   LYS B 240      7.922 -19.871  -9.607  1.00 23.06
BBBBATOM   4394  N   VAL B 241      6.075 -19.497  -8.378  1.00 23.98
BBBBATOM   4395  CA  VAL B 241      5.740 -20.911  -8.277  1.00 23.78
BBBBATOM   4396  CB  VAL B 241      5.858 -21.428  -6.833  1.00 24.03
BBBBATOM   4397  CG1 VAL B 241      5.548 -22.923  -6.803  1.00 24.14
BBBBATOM   4398  CG2 VAL B 241      7.242 -21.144  -6.281  1.00 23.49
BBBBATOM   4399  C   VAL B 241      4.299 -21.136  -8.723  1.00 24.15
BBBBATOM   4400  O   VAL B 241      3.380 -20.528  -8.184  1.00 24.63
BBBBATOM   4401  N   THR B 242      4.103 -22.000  -9.710  1.00 24.22
BBBBATOM   4402  CA  THR B 242      2.758 -22.301 -10.177  1.00 25.93
BBBBATOM   4403  CB  THR B 242      2.513 -21.812 -11.615  1.00 25.89
BBBBATOM   4404  OG1 THR B 242      3.466 -22.419 -12.492  1.00 27.48
BBBBATOM   4405  CG2 THR B 242      2.639 -20.299 -11.697  1.00 26.82
BBBBATOM   4406  C   THR B 242      2.555 -23.809, -10.135  1.00 26.29
BBBBATOM   4407  O   THR B 242      3.503 -24.577 -10.303  1.00 26.75
BBBBATOM   4408  N   GLU B 243      1.319 -24.228  -9.898  1.00 26.70
BBBBATOM   4409  CA  GLU B 243      0.999 -25.651  -9.837  1.00 27.03
BBBBATOM   4410  CB  GLU B 243     -0.473 -25.828  -9.445  1.00 29.00
BBBBATOM   4411  CG  GLU B 243     -0.831 -27.218  -8.962  1.00 30.88
BBBBATOM   4412  CD  GLU B 243     -2.297 -27.341  -8.583  1.00 33.00
BBBBATOM   4413  OE1 GLU B 243     -2.682 -28.402  -8.048  1.00 33.66
BBBBATOM   4414  OE2 GLU B 243     -3.063 -26.383  -8.827  1.00 32.17
BBBBATOM   4415  C   GLU B 243      1.256 -26.289 -11.202  1.00 26.61
BBBBATOM   4416  O   GLU B 243      1.841 -27.370 -11.304  1.00 26.48
BBBBATOM   4417  N   PHE B 244      0.807 -25.602 -12.248  1.00 26.54
BBBBATOM   4418  CA  PHE B 244      0.964 -26.068 -13.620  1.00 26.54
BBBBATOM   4419  CB  PHE B 244     -0.376 -26.553 -14.186  1.00 29.14
BBBBATOM   4420  CG  PHE B 244     -1.110 -27.531 -13.307  1.00 30.15
BBBBATOM   4421  CD1 PHE B 244     -0.622 -28.817 -13.107  1.00 32.26
BBBBATOM   4422  CD2 PHE B 244     -2.318 -27.172 -12.716  1.00 31.10
BBBBATOM   4423  CE1 PHE B 244     -1.335 -29.744 -12.328  1.00 33.63
BBBBATOM   4424  CE2 PHE B 244     -3.040 -28.083 -11.938  1.00 32.04
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BBBBATOM   4426  C   PHE B 244      1.420 -24.915 -14.507  1.00 25.60
BBBBATOM   4427  O   PHE B 244      1.604 -23.794 -14.053  1.00 24.93
BBBBATOM   4428  N   ILE B 245      1.591 -25.223 -15.786  1.00 27.02
BBBBATOM   4429  CA  ILE B 245      1.932 -24.242 -16.802  1.00 28.48
BBBBATOM   4430  CB  ILE B 245      3.441 -24.226 -17.159  1.00 28.41
BBBBATOM   4431  CG2 ILE B 245      3.676 -23.348 -18.399  1.00 27.05
BBBBATOM   4432  CG1 ILE B 245      4.245 -23.663 -15.983  1.00 27.10
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BBBBATOM   4434  C   ILE B 245      1.127 -24.721 -18.000  1.00 30.75
BBBBATOM   4435  O   ILE B 245      1.428 -25.753 -18.595  1.00 31.41
BBBBATOM   4436  N   ASP B 246      0.071 -23.997 -18.331  1.00 33.46
BBBBATOM   4437  CA  ASP B 246     -0.754 -24.396 -19.457  1.00 36.00
BBBBATOM   4438  CB  ASP B 246     -2.143 -23.754 -19.342  1.00 39.42
BBBBATOM   4439  CG  ASP B 246     -2.083 -22.246 -19.141  1.00 42.83
BBBBATOM   4440  OD1 ASP B 246     -1.447 -21.795 -18.162  1.00 44.54
BBBBATOM   4441  OD2 ASP B 246     -2.678 -21.511 -19.962  1.00 45.41
BBBBATOM   4442  C   ASP B 246     -0.088 -24.020 -20.780  1.00 35.70
BBBBATOM   4443  O   ASP B 246     -0.155 -24.768 -21.758  1.00 38.58
BBBBATOM   4444  N   ASP B 247      0.582 -22.876 -20.794  1.00 33.18
BBBBATOM   4445  CA  ASP B 247      1.245 -22.392 -21.999  1.00 30.74
BBBBATOM   4446  CB  ASP B 247      0.936 -20.904 -22.182  1.00 29.62
BBBBATOM   4447  CG  ASP B 247      1.344 -20.380 -23.548  1.00 30.15
BBBBATOM   4448  OD1 ASP B 247      2.161 -21.036 -24.225  1.00 27.57
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BBBBATOM	4449	OD2	ASP	B	247	0.854	-19.296	-23.935	1.00	29.19
BBBBATOM	4450	C	ASP	B	247	2.754	-22.607	-21.892	1.00	28.87
BBBBATOM	4451	O	ASP	B	247	3.494	-21.695	-21.525	1.00	27.28
BBBBATOM	4452	N	MET	B	248	3.204	-23.818	-22.205	1.00	27.72
BBBBATOM	4453	CA	MET	B	248	4.625	-24.136	-22.138	1.00	28.41
BBBBATOM	4454	CB	MET	B	248	4.856	-25.623	-22.405	1.00	29.48
BBBBATOM	4455	CG	MET	B	248	4.952	-26.469	-21.150	1.00	34.21
BBBBATOM	4456	SD	MET	B	248	6.277	-25.936	-20.049	1.00	38.21
BBBBATOM	4457	CE	MET	B	248	5.611	-26.499	-18.479	1.00	37.90
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BBBBATOM	4466	CA	ALA	B	250	5.188	-18.933	-23.390	1.00	21.78
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BBBBATOM	4471	CA	ALA	B	251	7.301	-20.259	-20.501	1.00	20.85
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BBBBATOM	4473	C	ALA	B	251	8.685	-20.512	-21.123	1.00	20.95
BBBBATOM	4474	O	ALA	B	251	9.689	-19.980	-20.648	1.00	21.14
BBBBATOM	4475	N	TYR	B	252	8.723	-21.314	-22.184	1.00	21.27
BBBBATOM	4476	CA	TYR	B	252	9.972	-21.616	-22.886	1.00	22.78
BBBBATOM	4477	CB	TYR	B	252	9.726	-22.661	-23.980	1.00	21.62
BBBBATOM	4478	CG	TYR	B	252	9.662	-24.100	-23.505	1.00	23.34
BBBBATOM	4479	CD1	TYR	B	252	9.003	-25.065	-24.261	1.00	22.88
BBBBATOM	4480	CE1	TYR	B	252	8.961	-26.392	-23.861	1.00	24.81
BBBBATOM	4481	CD2	TYR	B	252	10.288	-24.505	-22.319	1.00	22.30
BBBBATOM	4482	CE2	TYR	B	252	10.253	-25.838	-21.912	1.00	23.56
BBBBATOM	4483	CZ	TYR	B	252	9.590	-26.772	-22.687	1.00	24.26
BBBBATOM	4484	OH	TYR	B	252	9.554	-28.088	-22.305	1.00	25.57
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BBBBATOM	4490	C	ALA	B	253	10.783	-17.305	-23.617	1.00	23.30
BBBBATOM	4491	O	ALA	B	253	11.699	-16.546	-23.945	1.00	23.04
BBBBATOM	4492	N	TRP	B	254	10.299	-17.369	-22.379	1.00	20.49
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BBBBATOM	4500	NE1	TRP	B	254	11.185	-14.643	-17.226	1.00	20.30
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BBBBATOM	4508	CB	ALA	B	255	13.082	-20.507	-19.788	1.00	18.83
BBBBATOM	4509	C	ALA	B	255	14.737	-18.901	-20.713	1.00	18.88
BBBBATOM	4510	O	ALA	B	255	14.803	-18.688	-21.918	1.00	19.40
BBBBATOM	4511	N	ASP	B	256	15.803	-19.036	-19.927	1.00	19.01
BBBBATOM	4512	CA	ASP	B	256	17.176	-19.026	-20.434	1.00	17.58
BBBBATOM	4513	CB	ASP	B	256	18.078	-18.185	-19.534	1.00	18.47
BBBBATOM	4514	CG	ASP	B	256	17.954	-16.699	-19.795	1.00	18.05

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BBBBATOM   4515  OD1 ASP B 256      17.845 -15.944 -18.806  1.00 16.89
BBBBATOM   4516  OD2 ASP B 256      17.983 -16.287 -20.982  1.00 19.53
BBBBATOM   4517  C   ASP B 256      17.657 -20.481 -20.379  1.00 18.01
BBBBATOM   4518  O   ASP B 256      18.459 -20.929 -21.198  1.00 16.11
BBBBATOM   4519  N   VAL B 257      17.147 -21.216 -19.396  1.00 17.49
BBBBATOM   4520  CA  VAL B 257      17.535 -22.603 -19.194  1.00 18.53
BBBBATOM   4521  CB  VAL B 257      18.831 -22.681 -18.332  1.00 17.72
BBBBATOM   4522  CG1 VAL B 257      18.586 -22.069 -16.966  1.00 19.19
BBBBATOM   4523  CG2 VAL B 257      19.286 -24.129 -18.200  1.00 20.40
BBBBATOM   4524  C   VAL B 257      16.400 -23.363 -18.501  1.00 18.31
BBBBATOM   4525  O   VAL B 257      15.659 -22.795 -17.703  1.00 19.74
BBBBATOM   4526  N   VAL B 258      16.263 -24.643 -18.818  1.00 18.74
BBBBATOM   4527  CA  VAL B 258      15.208 -25.456 -18.234  1.00 19.32
BBBBATOM   4528  CB  VAL B 258      14.328 -26.100 -19.337  1.00 19.89
BBBBATOM   4529  CG1 VAL B 258      13.101 -26.754 -18.714  1.00 19.81
BBBBATOM   4530  CG2 VAL B 258      13.907 -25.041 -20.364  1.00 21.59
BBBBATOM   4531  C   VAL B 258      15.799 -26.585 -17.389  1.00 19.70
BBBBATOM   4532  O   VAL B 258      16.808 -27.175 -17.758  1.00 18.96
BBBBATOM   4533  N   VAL B 259      15.167 -26.861 -16.253  1.00 20.24
BBBBATOM   4534  CA  VAL B 259      15.581 -27.957 -15.374  1.00 19.85
BBBBATOM   4535  CB  VAL B 259      15.850 -27.483 -13.936  1.00 20.08
BBBBATOM   4536  CG1 VAL B 259      16.222 -28.689 -13.059  1.00 20.22
BBBBATOM   4537  CG2 VAL B 259      16.966 -26.453 -13.930  1.00 17.86
BBBBATOM   4538  C   VAL B 259      14.382 -28.890 -15.371  1.00 20.02
BBBBATOM   4539  O   VAL B 259      13.301 -28.500 -14.942  1.00 21.88
BBBBATOM   4540  N   CYS B 260      14.562 -30.111 -15.867  1.00 21.70
BBBBATOM   4541  CA  CYS B 260      13.454 -31.055 -15.946  1.00 22.00
BBBBATOM   4542  CB  CYS B 260      12.494 -30.618 -17.057  1.00 22.77
BBBBATOM   4543  SG  CYS B 260      13.297 -30.506 -18.711  1.00 22.15
BBBBATOM   4544  C   CYS B 260      13.903 -32.478 -16.242  1.00 21.86
BBBBATOM   4545  O   CYS B 260      15.087 -32.730 -16.496  1.00 21.34
BBBBATOM   4546  N   ARG B 261      12.937 -33.397 -16.212  1.00 22.34
BBBBATOM   4547  CA  ARG B 261      13.170 -34.800 -16.515  1.00 23.75
BBBBATOM   4548  CB  ARG B 261      11.964 -35.663 -16.104  1.00 27.16
BBBBATOM   4549  CG  ARG B 261      11.376 -35.337 -14.738  1.00 31.82
BBBBATOM   4550  CD  ARG B 261      11.490 -36.473 -13.732  1.00 36.33
BBBBATOM   4551  NE  ARG B 261      12.865 -36.721 -13.323  1.00 38.48
BBBBATOM   4552  CZ  ARG B 261      13.218 -37.176 -12.125  1.00 37.25
BBBBATOM   4553  NH1 ARG B 261      12.295 -37.433 -11.204  1.00 38.46
BBBBATOM   4554  NH2 ARG B 261      14.499 -37.370 -11.848  1.00 36.79
BBBBATOM   4555  C   ARG B 261      13.351 -34.871 -18.032  1.00 23.98
BBBBATOM   4556  O   ARG B 261      13.117 -33.883 -18.746  1.00 22.44
BBBBATOM   4557  N   SER B 262      13.740 -36.038 -18.527  1.00 22.00
BBBBATOM   4558  CA  SER B 262      13.975 -36.189 -19.948  1.00 23.18
BBBBATOM   4559  CB  SER B 262      15.481 -36.377 -20.203  1.00 24.45
BBBBATOM   4560  OG  SER B 262      16.043 -37.326 -19.311  1.00 25.79
BBBBATOM   4561  C   SER B 262      13.173 -37.263 -20.676  1.00 22.90
BBBBATOM   4562  O   SER B 262      13.738 -38.179 -21.274  1.00 23.25
BBBBATOM   4563  N   GLY B 263      11.850 -37.151 -20.619  1.00 22.74
BBBBATOM   4564  CA  GLY B 263      11.026 -38.079 -21.361  1.00 22.85
BBBBATOM   4565  C   GLY B 263      11.392 -37.793 -22.813  1.00 24.06
BBBBATOM   4566  O   GLY B 263      11.908 -36.705 -23.121  1.00 22.75
BBBBATOM   4567  N   ALA B 264      11.130 -38.739 -23.708  1.00 23.37
BBBBATOM   4568  CA  ALA B 264      11.482 -38.564 -25.115  1.00 24.25
BBBBATOM   4569  CB  ALA B 264      11.133 -39.829 -25.894  1.00 24.58
BBBBATOM   4570  C   ALA B 264      10.843 -37.343 -25.783  1.00 24.29
BBBBATOM   4571  O   ALA B 264      11.523 -36.572 -26.470  1.00 24.33
BBBBATOM   4572  N   LEU B 265       9.541 -37.167 -25.596  1.00 24.44
BBBBATOM   4573  CA  LEU B 265       8.846 -36.037 -26.205  1.00 24.66
BBBBATOM   4574  CB  LEU B 265       7.332 -36.183 -26.011  1.00 25.33
BBBBATOM   4575  CG  LEU B 265       6.760 -37.544 -26.426  1.00 27.97
BBBBATOM   4576  CD1 LEU B 265       5.242 -37.541 -26.258  1.00 28.21
BBBBATOM   4577  CD2 LEU B 265       7.146 -37.856 -27.878  1.00 27.40
BBBBATOM   4578  C   LEU B 265       9.331 -34.717 -25.613  1.00 24.47
BBBBATOM   4579  O   LEU B 265       9.374 -33.693 -26.301  1.00 23.85
BBBBATOM   4580  N   THR B 266       9.702 -34.747 -24.338  1.00 22.12
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BBBBATOM	4581	CA	THR	B	266	10.194	-33.557	-23.657	1.00 22.34
BBBBATOM	4582	CB	THR	B	266	10.348	-33.803	-22.140	1.00 22.35
BBBBATOM	4583	OG1	THR	B	266	9.061	-34.087	-21.583	1.00 24.46
BBBBATOM	4584	CG2	THR	B	266	10.945	-32.573	-21.444	1.00 24.00
BBBBATOM	4585	C	THR	B	266	11.535	-33.117	-24.226	1.00 21.15
BBBBATOM	4586	O	THR	B	266	11.761	-31.926	-24.442	1.00 20.35
BBBBATOM	4587	N	VAL	B	267	12.427	-34.075	-24.461	1.00 20.46
BBBBATOM	4588	CA	VAL	B	267	13.730	-33.762	-25.023	1.00 21.11
BBBBATOM	4589	CB	VAL	B	267	14.614	-35.039	-25.114	1.00 21.54
BBBBATOM	4590	CG1	VAL	B	267	15.903	-34.740	-25.865	1.00 20.72
BBBBATOM	4591	CG2	VAL	B	267	14.938	-35.541	-23.708	1.00 20.45
BBBBATOM	4592	C	VAL	B	267	13.548	-33.138	-26.416	1.00 21.34
BBBBATOM	4593	O	VAL	B	267	14.188	-32.135	-26.747	1.00 19.99
BBBBATOM	4594	N	SER	B	268	12.663	-33.717	-27.222	1.00 21.61
BBBBATOM	4595	CA	SER	B	268	12.411	-33.191	-28.567	1.00 21.96
BBBBATOM	4596	CB	SER	B	268	11.474	-34.121	-29.344	1.00 21.57
BBBBATOM	4597	OG	SER	B	268	12.141	-35.316	-29.721	1.00 24.06
BBBBATOM	4598	C	SER	B	268	11.817	-31.790	-28.519	1.00 21.81
BBBBATOM	4599	O	SER	B	268	12.158	-30.933	-29.336	1.00 22.60
BBBBATOM	4600	N	GLU	B	269	10.928	-31.563	-27.557	1.00 21.64
BBBBATOM	4601	CA	GLU	B	269	10.282	-30.272	-27.378	1.00 21.95
BBBBATOM	4602	CB	GLU	B	269	9.213	-30.399	-26.292	1.00 24.72
BBBBATOM	4603	CG	GLU	B	269	8.480	-29.128	-25.940	1.00 27.67
BBBBATOM	4604	CD	GLU	B	269	7.385	-29.380	-24.908	1.00 30.05
BBBBATOM	4605	OE1	GLU	B	269	6.325	-29.915	-25.287	1.00 31.50
BBBBATOM	4606	OE2	GLU	B	269	7.591	-29.057	-23.719	1.00 29.84
BBBBATOM	4607	C	GLU	B	269	11.321	-29.214	-26.999	1.00 21.68
BBBBATOM	4608	O	GLU	B	269	11.301	-28.095	-27.518	1.00 18.12
BBBBATOM	4609	N	ILE	B	270	12.224	-29.581	-26.092	1.00 19.43
BBBBATOM	4610	CA	ILE	B	270	13.295	-28.698	-25.638	1.00 20.62
BBBBATOM	4611	CB	ILE	B	270	14.157	-29.391	-24.533	1.00 20.30
BBBBATOM	4612	CG2	ILE	B	270	15.415	-28.595	-24.266	1.00 19.17
BBBBATOM	4613	CG1	ILE	B	270	13.337	-29.574	-23.254	1.00 21.32
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BBBBATOM	4615	C	ILE	B	270	14.214	-28.314	-26.806	1.00 20.58
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BBBBATOM	4617	N	ALA	B	271	14.574	-29.298	-27.624	1.00 21.29
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BBBBATOM	4620	C	ALA	B	271	14.766	-28.084	-29.745	1.00 23.03
BBBBATOM	4621	O	ALA	B	271	15.400	-27.156	-30.259	1.00 23.57
BBBBATOM	4622	N	ALA	B	272	13.479	-28.301	-29.988	1.00 21.81
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BBBBATOM	4624	CB	ALA	B	272	11.335	-28.053	-31.131	1.00 22.15
BBBBATOM	4625	C	ALA	B	272	12.590	-26.030	-30.355	1.00 22.78
BBBBATOM	4626	O	ALA	B	272	12.585	-25.058	-31.122	1.00 21.77
BBBBATOM	4627	N	ALA	B	273	12.474	-25.907	-29.034	1.00 21.06
BBBBATOM	4628	CA	ALA	B	273	12.361	-24.596	-28.407	1.00 21.97
BBBBATOM	4629	CB	ALA	B	273	11.919	-24.737	-26.949	1.00 20.63
BBBBATOM	4630	C	ALA	B	273	13.699	-23.867	-28.468	1.00 21.83
BBBBATOM	4631	O	ALA	B	273	13.754	-22.642	-28.344	1.00 22.67
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BBBBATOM	4639	CG	LEU	B	275	14.451	-22.870	-24.202	1.00 24.60
BBBBATOM	4640	CD1	LEU	B	275	13.220	-23.136	-23.349	1.00 26.44
BBBBATOM	4641	CD2	LEU	B	275	15.159	-21.609	-23.725	1.00 24.02
BBBBATOM	4642	C	LEU	B	275	17.698	-24.970	-24.318	1.00 18.79
BBBBATOM	4643	O	LEU	B	275	17.679	-26.180	-24.524	1.00 19.36
BBBBATOM	4644	N	PRO	B	276	18.634	-24.389	-23.554	1.00 17.27
BBBBATOM	4645	CD	PRO	B	276	18.925	-22.955	-23.416	1.00 16.95
BBBBATOM	4646	CA	PRO	B	276	19.651	-25.199	-22.875	1.00 16.62

BBBBATOM	4647	CB	PRO	B	276	20.619	-24.162	-22.317	1.00	17.27
BBBBATOM	4648	CG	PRO	B	276	20.408	-22.957	-23.195	1.00	18.59
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BBBBATOM	4657	CA	LEU	B	278	19.896	-29.429	-17.145	1.00	18.48
BBBBATOM	4658	CB	LEU	B	278	20.140	-28.619	-15.869	1.00	19.19
BBBBATOM	4659	CG	LEU	B	278	21.084	-29.308	-14.868	1.00	20.85
BBBBATOM	4660	CD1	LEU	B	278	21.283	-28.411	-13.668	1.00	21.11
BBBBATOM	4661	CD2	LEU	B	278	20.497	-30.647	-14.433	1.00	19.16
BBBBATOM	4662	C	LEU	B	278	18.884	-30.535	-16.898	1.00	19.62
BBBBATOM	4663	O	LEU	B	278	17.870	-30.330	-16.218	1.00	20.77
BBBBATOM	4664	N	PHE	B	279	19.149	-31.691	-17.495	1.00	19.50
BBBBATOM	4665	CA	PHE	B	279	18.266	-32.838	-17.392	1.00	21.59
BBBBATOM	4666	CB	PHE	B	279	18.385	-33.700	-18.651	1.00	21.07
BBBBATOM	4667	CG	PHE	B	279	17.740	-33.099	-19.876	1.00	19.35
BBBBATOM	4668	CD1	PHE	B	279	18.481	-32.898	-21.035	1.00	19.42
BBBBATOM	4669	CD2	PHE	B	279	16.379	-32.794	-19.888	1.00	18.16
BBBBATOM	4670	CE1	PHE	B	279	17.874	-32.405	-22.203	1.00	19.06
BBBBATOM	4671	CE2	PHE	B	279	15.759	-32.298	-21.052	1.00	17.65
BBBBATOM	4672	CZ	PHE	B	279	16.515	-32.108	-22.208	1.00	15.61
BBBBATOM	4673	C	PHE	B	279	18.525	-33.709	-16.167	1.00	22.86
BBBBATOM	4674	O	PHE	B	279	19.671	-34.065	-15.871	1.00	23.32
BBBBATOM	4675	N	VAL	B	280	17.445	-34.037	-15.461	1.00	23.88
BBBBATOM	4676	CA	VAL	B	280	17.502	-34.902	-14.281	1.00	25.67
BBBBATOM	4677	CB	VAL	B	280	16.883	-34.223	-13.048	1.00	26.89
BBBBATOM	4678	CG1	VAL	B	280	16.954	-35.159	-11.847	1.00	28.12
BBBBATOM	4679	CG2	VAL	B	280	17.631	-32.929	-12.742	1.00	27.70
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BBBBATOM	4681	O	VAL	B	280	15.509	-36.239	-14.346	1.00	24.57
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BBBBATOM	4683	CD	PRO	B	281	18.750	-37.057	-15.726	1.00	27.31
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BBBBATOM	4685	CB	PRO	B	281	17.851	-39.071	-16.492	1.00	29.44
BBBBATOM	4686	CG	PRO	B	281	18.791	-37.992	-16.895	1.00	29.67
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BBBBATOM	4693	CD1	PHE	B	282	11.720	-41.074	-12.130	1.00	41.80
BBBBATOM	4694	CD2	PHE	B	282	11.590	-42.886	-13.689	1.00	41.65
BBBBATOM	4695	CE1	PHE	B	282	10.975	-41.806	-11.209	1.00	42.03
BBBBATOM	4696	CE2	PHE	B	282	10.843	-43.628	-12.773	1.00	42.49
BBBBATOM	4697	CZ	PHE	B	282	10.536	-43.085	-11.532	1.00	41.74
BBBBATOM	4698	C	PHE	B	282	15.078	-41.776	-13.880	1.00	38.09
BBBBATOM	4699	O	PHE	B	282	15.357	-42.373	-14.921	1.00	38.33
BBBBATOM	4700	N	GLN	B	283	15.492	-42.197	-12.690	1.00	39.70
BBBBATOM	4701	CA	GLN	B	283	16.319	-43.395	-12.591	1.00	41.11
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BBBBATOM	4705	OE1	GLN	B	283	20.199	-44.068	-11.712	1.00	43.66
BBBBATOM	4706	NE2	GLN	B	283	18.969	-45.135	-13.254	1.00	42.46
BBBBATOM	4707	C	GLN	B	283	15.543	-44.679	-12.846	1.00	41.60
BBBBATOM	4708	O	GLN	B	283	14.382	-44.809	-12.462	1.00	40.91
BBBBATOM	4709	N	HIS	B	284	16.211	-45.618	-13.511	1.00	42.92
BBBBATOM	4710	CA	HIS	B	284	15.641	-46.917	-13.843	1.00	43.69
BBBBATOM	4711	CB	HIS	B	284	14.508	-46.760	-14.858	1.00	43.91
BBBBATOM	4712	CG	HIS	B	284	13.795	-48.039	-15.165	1.00	44.71

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BBBBATOM   4713  CD2 HIS B 284      12.574 -48.489 -14.793  1.00 44.80
BBBBATOM   4714  ND1 HIS B 284      14.360 -49.044 -15.923  1.00 44.69
BBBBATOM   4715  CE1 HIS B 284      13.516 -50.058 -16.002  1.00 45.06
BBBBATOM   4716  NE2 HIS B 284      12.425 -49.747 -15.325  1.00 44.90
BBBBATOM   4717  C   HIS B 284      16.749 -47.788 -14.424  1.00 44.09
BBBBATOM   4718  O   HIS B 284      17.602 -47.302 -15.164  1.00 43.02
BBBBATOM   4719  N   LYS B 285      16.740 -49.074 -14.085  1.00 44.90
BBBBATOM   4720  CA  LYS B 285      17.767 -49.993 -14.571  1.00 45.34
BBBBATOM   4721  CB  LYS B 285      17.386 -51.436 -14.222  1.00 46.84
BBBBATOM   4722  CG  LYS B 285      18.541 -52.425 -14.327  1.00 49.53
BBBBATOM   4723  CD  LYS B 285      18.140 -53.802 -13.807  1.00 51.08
BBBBATOM   4724  CE  LYS B 285      19.325 -54.759 -13.780  1.00 51.58
BBBBATOM   4725  NZ  LYS B 285      18.931 -56.115 -13.292  1.00 52.11
BBBBATOM   4726  C   LYS B 285      17.969 -49.853 -16.079  1.00 45.02
BBBBATOM   4727  O   LYS B 285      19.067 -50.070 -16.595  1.00 45.49
BBBBATOM   4728  N   ASP B 286      16.903 -49.478 -16.777  1.00 44.33
BBBBATOM   4729  CA  ASP B 286      16.949 -49.299 -18.222  1.00 43.26
BBBBATOM   4730  CB  ASP B 286      15.532 -49.379 -18.794  1.00 45.91
BBBBATOM   4731  CG  ASP B 286      15.511 -49.354 -20.304  1.00 48.32
BBBBATOM   4732  OD1 ASP B 286      15.971 -50.338 -20.925  1.00 49.52
BBBBATOM   4733  OD2 ASP B 286      15.037 -48.346 -20.872  1.00 51.04
BBBBATOM   4734  C   ASP B 286      17.573 -47.947 -18.582  1.00 40.92
BBBBATOM   4735  O   ASP B 286      18.179 -47.796 -19.643  1.00 40.31
BBBBATOM   4736  N   ARG B 287      17.415 -46.972 -17.689  1.00 38.60
BBBBATOM   4737  CA  ARG B 287      17.951 -45.623 -17.883  1.00 36.28
BBBBATOM   4738  CB  ARG B 287      19.477 -45.650 -17.910  1.00 37.28
BBBBATOM   4739  CG  ARG B 287      20.116 -46.263 -16.687  1.00 40.54
BBBBATOM   4740  CD  ARG B 287      21.605 -46.395 -16.906  1.00 42.34
BBBBATOM   4741  NE  ARG B 287      22.291 -45.113 -16.802  1.00 44.33
BBBBATOM   4742  CZ  ARG B 287      23.449 -44.842 -17.392  1.00 45.20
BBBBATOM   4743  NH1 ARG B 287      24.045 -45.764 -18.135  1.00 45.60
BBBBATOM   4744  NH2 ARG B 287      24.019 -43.656 -17.227  1.00 45.68
BBBBATOM   4745  C   ARG B 287      17.449 -45.005 -19.180  1.00 33.59
BBBBATOM   4746  O   ARG B 287      18.167 -44.255 -19.844  1.00 32.61
BBBBATOM   4747  N   GLN B 288      16.212 -45.321 -19.533  1.00 30.94
BBBBATOM   4748  CA  GLN B 288      15.622 -44.804 -20.755  1.00 30.77
BBBBATOM   4749  CB  GLN B 288      14.143 -45.158 -20.810  1.00 30.59
BBBBATOM   4750  CG  GLN B 288      13.473 -44.772 -22.109  1.00 29.73
BBBBATOM   4751  CD  GLN B 288      11.981 -44.971 -22.044  1.00 28.04
BBBBATOM   4752  OE1 GLN B 288      11.294 -44.295 -21.279  1.00 29.59
BBBBATOM   4753  NE2 GLN B 288      11.468 -45.905 -22.838  1.00 26.98
BBBBATOM   4754  C   GLN B 288      15.783 -43.291 -20.885  1.00 29.70
BBBBATOM   4755  O   GLN B 288      16.268 -42.801 -21.902  1.00 29.79
BBBBATOM   4756  N   GLN B 289      15.378 -42.554 -19.857  1.00 29.38
BBBBATOM   4757  CA  GLN B 289      15.474 -41.099 -19.904  1.00 29.46
BBBBATOM   4758  CB  GLN B 289      14.772 -40.472 -18.700  1.00 29.25
BBBBATOM   4759  CG  GLN B 289      13.265 -40.416 -18.883  1.00 29.32
BBBBATOM   4760  CD  GLN B 289      12.575 -39.585 -17.826  1.00 29.84
BBBBATOM   4761  OE1 GLN B 289      13.191 -38.728 -17.188  1.00 29.52
BBBBATOM   4762  NE2 GLN B 289      11.281 -39.821 -17.647  1.00 28.95
BBBBATOM   4763  C   GLN B 289      16.906 -40.613 -20.005  1.00 29.36
BBBBATOM   4764  O   GLN B 289      17.173 -39.557 -20.585  1.00 29.12
BBBBATOM   4765  N   TYR B 290      17.835 -41.374 -19.442  1.00 28.95
BBBBATOM   4766  CA  TYR B 290      19.228 -40.984 -19.550  1.00 29.55
BBBBATOM   4767  CB  TYR B 290      20.136 -41.934 -18.768  1.00 31.40
BBBBATOM   4768  CG  TYR B 290      21.587 -41.780 -19.148  1.00 33.37
BBBBATOM   4769  CD1 TYR B 290      22.332 -40.682 -18.717  1.00 34.57
BBBBATOM   4770  CE1 TYR B 290      23.644 -40.490 -19.148  1.00 35.97
BBBBATOM   4771  CD2 TYR B 290      22.192 -42.684 -20.017  1.00 34.90
BBBBATOM   4772  CE2 TYR B 290      23.497 -42.500 -20.453  1.00 36.03
BBBBATOM   4773  CZ  TYR B 290      24.214 -41.402 -20.019  1.00 36.29
BBBBATOM   4774  OH  TYR B 290      25.499 -41.215 -20.475  1.00 39.44
BBBBATOM   4775  C   TYR B 290      19.593 -41.042 -21.032  1.00 28.80
BBBBATOM   4776  O   TYR B 290      20.192 -40.113 -21.567  1.00 29.22
BBBBATOM   4777  N   TRP B 291      19.227 -42.135 -21.697  1.00 27.57
BBBBATOM   4778  CA  TRP B 291      19.542 -42.282 -23.116  1.00 28.07
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BBBBATOM	4779	CB	TRP	B	291	19.217	-43.705	-23.599	1.00	29.42
BBBBATOM	4780	CG	TRP	B	291	20.070	-44.750	-22.936	1.00	31.82
BBBBATOM	4781	CD2	TRP	B	291	21.487	-44.908	-23.069	1.00	33.22
BBBBATOM	4782	CE2	TRP	B	291	21.873	-45.966	-22.213	1.00	33.81
BBBBATOM	4783	CE3	TRP	B	291	22.470	-44.257	-23.826	1.00	33.13
BBBBATOM	4784	CD1	TRP	B	291	19.663	-45.695	-22.035	1.00	32.62
BBBBATOM	4785	NE1	TRP	B	291	20.741	-46.428	-21.595	1.00	33.43
BBBBATOM	4786	CZ2	TRP	B	291	23.203	-46.387	-22.093	1.00	34.69
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BBBBATOM	4788	CH2	TRP	B	291	24.146	-45.732	-22.845	1.00	35.26
BBBBATOM	4789	C	TRP	B	291	18.808	-41.256	-23.978	1.00	26.84
BBBBATOM	4790	O	TRP	B	291	19.283	-40.900	-25.058	1.00	26.55
BBBBATOM	4791	N	ASN	B	292	17.658	-40.779	-23.508	1.00	25.52
BBBBATOM	4792	CA	ASN	B	292	16.902	-39.784	-24.270	1.00	26.06
BBBBATOM	4793	CB	ASN	B	292	15.484	-39.599	-23.709	1.00	24.78
BBBBATOM	4794	CG	ASN	B	292	14.590	-40.811	-23.928	1.00	24.46
BBBBATOM	4795	OD1	ASN	B	292	14.842	-41.641	-24.798	1.00	25.33
BBBBATOM	4796	ND2	ASN	B	292	13.523	-40.900	-23.146	1.00	23.83
BBBBATOM	4797	C	ASN	B	292	17.605	-38.427	-24.258	1.00	25.99
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BBBBATOM	4799	N	ALA	B	293	18.242	-38.105	-23.139	1.00	25.66
BBBBATOM	4800	CA	ALA	B	293	18.926	-36.822	-22.979	1.00	25.69
BBBBATOM	4801	CB	ALA	B	293	18.940	-36.422	-21.506	1.00	24.17
BBBBATOM	4802	C	ALA	B	293	20.346	-36.800	-23.521	1.00	25.67
BBBBATOM	4803	O	ALA	B	293	20.855	-35.743	-23.902	1.00	25.52
BBBBATOM	4804	N	LEU	B	294	20.978	-37.969	-23.560	1.00	25.62
BBBBATOM	4805	CA	LEU	B	294	22.354	-38.088	-24.032	1.00	25.90
BBBBATOM	4806	CB	LEU	B	294	22.745	-39.566	-24.121	1.00	26.51
BBBBATOM	4807	CG	LEU	B	294	24.226	-39.864	-24.350	1.00	28.12
BBBBATOM	4808	CD1	LEU	B	294	25.085	-39.055	-23.380	1.00	28.29
BBBBATOM	4809	CD2	LEU	B	294	24.470	-41.368	-24.169	1.00	28.15
BBBBATOM	4810	C	LEU	B	294	22.644	-37.392	-25.359	1.00	25.66
BBBBATOM	4811	O	LEU	B	294	23.677	-36.741	-25.507	1.00	24.79
BBBBATOM	4812	N	PRO	B	295	21.748	-37.532	-26.351	1.00	26.24
BBBBATOM	4813	CD	PRO	B	295	20.560	-38.400	-26.437	1.00	25.75
BBBBATOM	4814	CA	PRO	B	295	21.998	-36.870	-27.635	1.00	26.15
BBBBATOM	4815	CB	PRO	B	295	20.740	-37.201	-28.439	1.00	26.70
BBBBATOM	4816	CG	PRO	B	295	20.382	-38.548	-27.932	1.00	26.84
BBBBATOM	4817	C	PRO	B	295	22.219	-35.358	-27.480	1.00	25.78
BBBBATOM	4818	O	PRO	B	295	23.138	-34.792	-28.069	1.00	25.05
BBBBATOM	4819	N	LEU	B	296	21.375	-34.703	-26.688	1.00	25.66
BBBBATOM	4820	CA	LEU	B	296	21.521	-33.265	-26.481	1.00	25.42
BBBBATOM	4821	CB	LEU	B	296	20.283	-32.685	-25.779	1.00	24.45
BBBBATOM	4822	CG	LEU	B	296	19.066	-32.458	-26.679	1.00	25.59
BBBBATOM	4823	CD1	LEU	B	296	17.968	-31.718	-25.911	1.00	23.56
BBBBATOM	4824	CD2	LEU	B	296	19.496	-31.630	-27.893	1.00	25.87
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BBBBATOM	4826	O	LEU	B	296	23.435	-31.917	-25.944	1.00	25.26
BBBBATOM	4827	N	GLU	B	297	23.143	-33.785	-24.730	1.00	26.14
BBBBATOM	4828	CA	GLU	B	297	24.354	-33.530	-23.953	1.00	28.78
BBBBATOM	4829	CB	GLU	B	297	24.470	-34.483	-22.755	1.00	29.05
BBBBATOM	4830	CG	GLU	B	297	25.716	-34.210	-21.908	1.00	30.81
BBBBATOM	4831	CD	GLU	B	297	25.812	-35.087	-20.671	1.00	31.84
BBBBATOM	4832	OE1	GLU	B	297	25.655	-34.555	-19.551	1.00	31.74
BBBBATOM	4833	OE2	GLU	B	297	26.045	-36.307	-20.820	1.00	31.56
BBBBATOM	4834	C	GLU	B	297	25.577	-33.686	-24.846	1.00	29.06
BBBBATOM	4835	O	GLU	B	297	26.528	-32.910	-24.746	1.00	29.11
BBBBATOM	4836	N	LYS	B	298	25.543	-34.688	-25.722	1.00	31.21
BBBBATOM	4837	CA	LYS	B	298	26.644	-34.947	-26.648	1.00	31.90
BBBBATOM	4838	CB	LYS	B	298	26.379	-36.216	-27.464	1.00	33.65
BBBBATOM	4839	CG	LYS	B	298	26.519	-37.514	-26.680	1.00	36.05
BBBBATOM	4840	CD	LYS	B	298	26.251	-38.734	-27.568	1.00	37.69
BBBBATOM	4841	CE	LYS	B	298	26.461	-40.033	-26.801	1.00	38.51
BBBBATOM	4842	NZ	LYS	B	298	26.094	-41.235	-27.607	1.00	39.05
BBBBATOM	4843	C	LYS	B	298	26.829	-33.768	-27.598	1.00	31.69
BBBBATOM	4844	O	LYS	B	298	27.945	-33.455	-27.998	1.00	30.87

BBBBATOM	4845	N	ALA	B	299	25.725	-33.116	-27.952	1.00	31.63
BBBBATOM	4846	CA	ALA	B	299	25.773	-31.965	-28.847	1.00	30.38
BBBBATOM	4847	CB	ALA	B	299	24.415	-31.778	-29.521	1.00	30.22
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BBBBATOM	4851	CA	GLY	B	300	26.777	-29.635	-26.017	1.00	26.18
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BBBBATOM	4864	N	LYS	B	303	23.156	-30.613	-20.009	1.00	24.62
BBBBATOM	4865	CA	LYS	B	303	23.979	-31.340	-19.048	1.00	25.86
BBBBATOM	4866	CB	LYS	B	303	24.632	-30.401	-18.036	1.00	27.85
BBBBATOM	4867	CG	LYS	B	303	25.466	-31.146	-16.986	1.00	29.37
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BBBBATOM	4870	NZ	LYS	B	303	27.827	-29.952	-14.181	1.00	33.62
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BBBBATOM	4872	O	LYS	B	303	22.015	-31.948	-17.802	1.00	25.76
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BBBBATOM	4874	CA	ILE	B	304	22.753	-34.598	-17.550	1.00	27.17
BBBBATOM	4875	CB	ILE	B	304	22.786	-35.946	-18.316	1.00	27.06
BBBBATOM	4876	CG2	ILE	B	304	21.977	-36.996	-17.555	1.00	28.49
BBBBATOM	4877	CG1	ILE	B	304	22.242	-35.769	-19.733	1.00	27.61
BBBBATOM	4878	CD1	ILE	B	304	22.380	-37.009	-20.599	1.00	27.05
BBBBATOM	4879	C	ILE	B	304	23.308	-34.855	-16.160	1.00	27.00
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BBBBATOM	4881	N	ILE	B	305	22.428	-34.869	-15.168	1.00	27.22
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BBBBATOM	4883	CB	ILE	B	305	22.713	-33.977	-12.858	1.00	28.91
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BBBBATOM	4886	CD1	ILE	B	305	23.674	-31.653	-12.367	1.00	29.43
BBBBATOM	4887	C	ILE	B	305	21.934	-36.302	-13.351	1.00	29.64
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BBBBATOM	4892	CG	GLU	B	306	22.529	-40.067	-15.035	1.00	36.39
BBBBATOM	4893	CD	GLU	B	306	23.114	-41.388	-15.504	1.00	36.86
BBBBATOM	4894	OE1	GLU	B	306	22.468	-42.433	-15.289	1.00	36.59
BBBBATOM	4895	OE2	GLU	B	306	24.214	-41.378	-16.099	1.00	37.75
BBBBATOM	4896	C	GLU	B	306	21.531	-38.704	-11.552	1.00	35.50
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BBBBATOM	4898	N	GLN	B	307	20.612	-39.514	-11.048	1.00	38.41
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BBBBATOM	4900	CB	GLN	B	307	19.397	-40.734	-9.322	1.00	40.99
BBBBATOM	4901	CG	GLN	B	307	18.896	-40.769	-7.896	1.00	42.76
BBBBATOM	4902	CD	GLN	B	307	17.879	-41.867	-7.681	1.00	44.33
BBBBATOM	4903	OE1	GLN	B	307	18.181	-43.051	-7.847	1.00	44.46
BBBBATOM	4904	NE2	GLN	B	307	16.659	-41.481	-7.318	1.00	45.30
BBBBATOM	4905	C	GLN	B	307	21.647	-39.784	-8.776	1.00	40.94
BBBBATOM	4906	O	GLN	B	307	21.796	-39.154	-7.732	1.00	41.24
BBBBATOM	4907	N	PRO	B	308	22.580	-40.648	-9.224	1.00	42.16
BBBBATOM	4908	CD	PRO	B	308	22.456	-41.593	-10.349	1.00	42.40
BBBBATOM	4909	CA	PRO	B	308	23.828	-40.891	-8.484	1.00	43.20
BBBBATOM	4910	CB	PRO	B	308	24.533	-41.954	-9.329	1.00	43.16

BBBBATOM	4911	CG	PRO	B	308	23.395	-42.708	-9.938	1.00	43.10
BBBBATOM	4912	C	PRO	B	308	24.719	-39.668	-8.250	1.00	43.82
BBBBATOM	4913	O	PRO	B	308	25.652	-39.724	-7.449	1.00	44.24
BBBBATOM	4914	N	GLN	B	309	24.442	-38.569	-8.944	1.00	44.04
BBBBATOM	4915	CA	GLN	B	309	25.247	-37.361	-8.787	1.00	43.46
BBBBATOM	4916	CB	GLN	B	309	26.071	-37.104	-10.056	1.00	44.98
BBBBATOM	4917	CG	GLN	B	309	27.183	-38.113	-10.329	1.00	46.93
BBBBATOM	4918	CD	GLN	B	309	26.683	-39.437	-10.885	1.00	47.93
BBBBATOM	4919	OE1	GLN	B	309	27.459	-40.376	-11.054	1.00	48.87
BBBBATOM	4920	NE2	GLN	B	309	25.388	-39.515	-11.179	1.00	49.17
BBBBATOM	4921	C	GLN	B	309	24.417	-36.119	-8.479	1.00	42.87
BBBBATOM	4922	O	GLN	B	309	24.955	-35.013	-8.404	1.00	43.33
BBBBATOM	4923	N	LEU	B	310	23.113	-36.297	-8.289	1.00	41.06
BBBBATOM	4924	CA	LEU	B	310	22.232	-35.166	-8.022	1.00	39.65
BBBBATOM	4925	CB	LEU	B	310	20.779	-35.549	-8.330	1.00	39.95
BBBBATOM	4926	CG	LEU	B	310	19.730	-34.437	-8.480	1.00	39.98
BBBBATOM	4927	CD1	LEU	B	310	19.545	-33.699	-7.166	1.00	41.39
BBBBATOM	4928	CD2	LEU	B	310	20.160	-33.472	-9.580	1.00	40.19
BBBBATOM	4929	C	LEU	B	310	22.342	-34.659	-6.591	1.00	38.83
BBBBATOM	4930	O	LEU	B	310	22.246	-35.428	-5.634	1.00	39.25
BBBBATOM	4931	N	SER	B	311	22.541	-33.354	-6.457	1.00	36.17
BBBBATOM	4932	CA	SER	B	311	22.660	-32.714	-5.154	1.00	34.90
BBBBATOM	4933	CB	SER	B	311	24.059	-32.928	-4.569	1.00	35.08
BBBBATOM	4934	OG	SER	B	311	25.022	-32.135	-5.248	1.00	33.92
BBBBATOM	4935	C	SER	B	311	22.434	-31.227	-5.357	1.00	33.51
BBBBATOM	4936	O	SER	B	311	22.476	-30.741	-6.485	1.00	33.60
BBBBATOM	4937	N	VAL	B	312	22.202	-30.509	-4.266	1.00	32.42
BBBBATOM	4938	CA	VAL	B	312	21.990	-29.074	-4.341	1.00	31.50
BBBBATOM	4939	CB	VAL	B	312	21.707	-28.482	-2.938	1.00	31.69
BBBBATOM	4940	CG1	VAL	B	312	21.546	-26.976	-3.023	1.00	31.54
BBBBATOM	4941	CG2	VAL	B	312	20.445	-29.106	-2.362	1.00	31.93
BBBBATOM	4942	C	VAL	B	312	23.228	-28.417	-4.946	1.00	31.40
BBBBATOM	4943	O	VAL	B	312	23.123	-27.612	-5.875	1.00	30.04
BBBBATOM	4944	N	ASP	B	313	24.406	-28.780	-4.444	1.00	30.18
BBBBATOM	4945	CA	ASP	B	313	25.642	-28.202	-4.957	1.00	29.61
BBBBATOM	4946	CB	ASP	B	313	26.840	-28.656	-4.120	1.00	32.36
BBBBATOM	4947	CG	ASP	B	313	26.817	-28.085	-2.718	1.00	34.21
BBBBATOM	4948	OD1	ASP	B	313	26.662	-26.855	-2.578	1.00	36.52
BBBBATOM	4949	OD2	ASP	B	313	26.958	-28.865	-1.751	1.00	38.92
BBBBATOM	4950	C	ASP	B	313	25.910	-28.516	-6.425	1.00	28.84
BBBBATOM	4951	O	ASP	B	313	26.442	-27.677	-7.146	1.00	28.96
BBBBATOM	4952	N	ALA	B	314	25.555	-29.719	-6.868	1.00	26.61
BBBBATOM	4953	CA	ALA	B	314	25.782	-30.099	-8.254	1.00	26.47
BBBBATOM	4954	CB	ALA	B	314	25.441	-31.575	-8.460	1.00	26.05
BBBBATOM	4955	C	ALA	B	314	24.928	-29.220	-9.174	1.00	25.78
BBBBATOM	4956	O	ALA	B	314	25.412	-28.714	-10.187	1.00	24.94
BBBBATOM	4957	N	VAL	B	315	23.661	-29.046	-8.815	1.00	25.00
BBBBATOM	4958	CA	VAL	B	315	22.755	-28.215	-9.612	1.00	25.33
BBBBATOM	4959	CB	VAL	B	315	21.305	-28.298	-9.088	1.00	24.74
BBBBATOM	4960	CG1	VAL	B	315	20.392	-27.382	-9.898	1.00	23.53
BBBBATOM	4961	CG2	VAL	B	315	20.810	-29.738	-9.172	1.00	25.69
BBBBATOM	4962	C	VAL	B	315	23.222	-26.764	-9.561	1.00	25.02
BBBBATOM	4963	O	VAL	B	315	23.398	-26.125	-10.590	1.00	25.73
BBBBATOM	4964	N	ALA	B	316	23.445	-26.251	-8.359	1.00	26.04
BBBBATOM	4965	CA	ALA	B	316	23.888	-24.872	-8.199	1.00	27.13
BBBBATOM	4966	CB	ALA	B	316	24.059	-24.545	-6.714	1.00	27.12
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BBBBATOM	4971	CB	ASN	B	317	28.493	-26.271	-9.081	1.00	31.30
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BBBBATOM	4974	ND2	ASN	B	317	29.170	-27.171	-6.933	1.00	35.63
BBBBATOM	4975	C	ASN	B	317	27.270	-25.310	-11.026	1.00	27.23
BBBBATOM	4976	O	ASN	B	317	27.887	-24.543	-11.765	1.00	26.36

BBBBATOM	4977	N	THR	B	318	26.424	-26.224	-11.482	1.00	26.95
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BBBBATOM	4989	CD2	LEU	B	319	20.963	-24.065	-14.237	1.00	22.39
BBBBATOM	4990	C	LEU	B	319	24.814	-22.169	-13.253	1.00	25.23
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BBBBATOM	4995	C	ALA	B	320	27.549	-20.865	-13.010	1.00	24.21
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BBBBATOM	4999	C	GLY	B	321	28.509	-21.642	-15.993	1.00	24.34
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BBBBATOM	5002	CA	TRP	B	322	26.738	-21.007	-17.521	1.00	21.72
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BBBBATOM	5005	CD2	TRP	B	322	24.789	-24.370	-17.939	1.00	19.16
BBBBATOM	5006	CE2	TRP	B	322	25.479	-25.584	-18.164	1.00	20.31
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BBBBATOM	5013	C	TRP	B	322	26.422	-19.524	-17.722	1.00	21.61
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BBBBATOM	5022	CA	ARG	B	324	24.725	-15.741	-21.112	1.00	18.09
BBBBATOM	5023	CB	ARG	B	324	24.298	-14.268	-21.108	1.00	19.15
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BBBBATOM	5025	CD	ARG	B	324	22.508	-12.662	-20.220	1.00	22.13
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BBBBATOM	5027	CZ	ARG	B	324	20.268	-13.403	-19.510	1.00	21.63
BBBBATOM	5028	NH1	ARG	B	324	20.206	-14.224	-20.549	1.00	20.63
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BBBBATOM	5030	C	ARG	B	324	25.288	-16.145	-22.481	1.00	17.79
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BBBBATOM	5038	OE2	GLU	B	325	31.408	-15.325	-24.615	1.00	20.56
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BBBBATOM	5042	CA	THR	B	326	27.460	-20.055	-23.070	1.00	16.39

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BBBBATOM   5050  CB  LEU B 327      22.791 -19.514 -21.791  1.00 17.35
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BBBBATOM   5052  CD1 LEU B 327      22.192 -18.930 -19.416  1.00 14.82
BBBBATOM   5053  CD2 LEU B 327      22.361 -21.312 -20.129  1.00 18.13
BBBBATOM   5054  C   LEU B 327      23.145 -20.096 -24.198  1.00 17.58
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BBBBATOM   5057  CA  LEU B 328      23.175 -18.745 -26.222  1.00 17.39
BBBBATOM   5058  CB  LEU B 328      23.706 -17.379 -26.690  1.00 17.84
BBBBATOM   5059  CG  LEU B 328      23.475 -17.021 -28.173  1.00 18.65
BBBBATOM   5060  CD1 LEU B 328      21.988 -17.112 -28.494  1.00 16.92
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BBBBATOM   5063  O   LEU B 328      23.003 -20.400 -27.953  1.00 17.59
BBBBATOM   5064  N   THR B 329      24.977 -20.244 -26.910  1.00 20.12
BBBBATOM   5065  CA  THR B 329      25.567 -21.335 -27.688  1.00 21.30
BBBBATOM   5066  CB  THR B 329      27.069 -21.556 -27.336  1.00 22.69
BBBBATOM   5067  OG1 THR B 329      27.866 -20.591 -28.029  1.00 25.80
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BBBBATOM   5070  O   THR B 329      24.552 -23.382 -28.398  1.00 20.34
BBBBATOM   5071  N   MET B 330      24.494 -22.933 -26.200  1.00 20.31
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BBBBATOM   5076  CE  MET B 330      24.118 -26.250 -21.622  1.00 22.37
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BBBBATOM   5078  O   MET B 330      21.924 -25.167 -27.029  1.00 20.85
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BBBBATOM   5087  CG  GLU B 332      22.328 -20.455 -31.143  1.00 24.10
BBBBATOM   5088  CD  GLU B 332      23.428 -19.522 -31.572  1.00 26.61
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BBBBATOM   5095  CB  ARG B 333      24.117 -26.789 -29.427  1.00 25.03
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BBBBATOM   5099  CZ  ARG B 333      28.772 -26.001 -27.932  1.00 30.32
BBBBATOM   5100  NH1 ARG B 333      28.514 -26.361 -26.678  1.00 32.07
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BBBBATOM   5103  O   ARG B 333      21.548 -28.151 -30.895  1.00 23.45
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BBBBATOM   5105  CA  ALA B 334      19.648 -27.420 -29.063  1.00 22.89
BBBBATOM   5106  CB  ALA B 334      18.915 -26.800 -27.882  1.00 22.08
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BBBBATOM	5110	CA	ARG	B	335	17.795	-25.892	-32.002	1.00	23.54
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BBBBATOM	5141	CD1	ILE	B	339	15.688	-35.378	-36.667	1.00	37.71
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BBBBATOM	5149	C	PRO	B	340	9.551	-30.409	-37.284	1.00	34.07
BBBBATOM	5150	O	PRO	B	340	8.410	-30.222	-36.861	1.00	34.18
BBBBATOM	5151	N	ASP	B	341	9.803	-31.180	-38.334	1.00	33.42
BBBBATOM	5152	CA	ASP	B	341	8.711	-31.820	-39.056	1.00	33.33
BBBBATOM	5153	CB	ASP	B	341	8.802	-31.448	-40.536	1.00	35.03
BBBBATOM	5154	CG	ASP	B	341	10.101	-31.886	-41.159	1.00	37.02
BBBBATOM	5155	OD1	ASP	B	341	11.125	-31.907	-40.443	1.00	37.17
BBBBATOM	5156	OD2	ASP	B	341	10.102	-32.200	-42.367	1.00	40.57
BBBBATOM	5157	C	ASP	B	341	8.655	-33.336	-38.899	1.00	32.11
BBBBATOM	5158	O	ASP	B	341	8.377	-34.066	-39.854	1.00	30.74
BBBBATOM	5159	N	ALA	B	342	8.908	-33.807	-37.683	1.00	30.63
BBBBATOM	5160	CA	ALA	B	342	8.875	-35.238	-37.411	1.00	29.09
BBBBATOM	5161	CB	ALA	B	342	9.174	-35.496	-35.927	1.00	28.28
BBBBATOM	5162	C	ALA	B	342	7.530	-35.844	-37.792	1.00	28.32
BBBBATOM	5163	O	ALA	B	342	7.475	-36.901	-38.416	1.00	29.88
BBBBATOM	5164	N	THR	B	343	6.441	-35.177	-37.427	1.00	28.28
BBBBATOM	5165	CA	THR	B	343	5.115	-35.696	-37.744	1.00	28.55
BBBBATOM	5166	CB	THR	B	343	3.998	-34.765	-37.205	1.00	29.04
BBBBATOM	5167	OG1	THR	B	343	4.119	-34.642	-35.782	1.00	28.04
BBBBATOM	5168	CG2	THR	B	343	2.628	-35.330	-37.528	1.00	28.54
BBBBATOM	5169	C	THR	B	343	4.934	-35.882	-39.254	1.00	29.50
BBBBATOM	5170	O	THR	B	343	4.533	-36.952	-39.711	1.00	28.08
BBBBATOM	5171	N	GLU	B	344	5.234	-34.843	-40.030	1.00	30.76
BBBBATOM	5172	CA	GLU	B	344	5.085	-34.933	-41.480	1.00	32.00
BBBBATOM	5173	CB	GLU	B	344	5.414	-33.589	-42.142	1.00	34.02
BBBBATOM	5174	CG	GLU	B	344	4.412	-32.483	-41.814	1.00	38.27

BBBBATOM	5175	CD	GLU	B	344	4.807	-31.661	-40.594	1.00	40.96
BBBBATOM	5176	OE1	GLU	B	344	5.252	-32.252	-39.582	1.00	41.33
BBBBATOM	5177	OE2	GLU	B	344	4.665	-30.419	-40.649	1.00	42.30
BBBBATOM	5178	C	GLU	B	344	5.970	-36.032	-42.056	1.00	31.14
BBBBATOM	5179	O	GLU	B	344	5.534	-36.805	-42.909	1.00	32.33
BBBBATOM	5180	N	ARG	B	345	7.209	-36.106	-41.587	1.00	30.66
BBBBATOM	5181	CA	ARG	B	345	8.138	-37.123	-42.067	1.00	31.44
BBBBATOM	5182	CB	ARG	B	345	9.494	-36.986	-41.376	1.00	33.54
BBBBATOM	5183	CG	ARG	B	345	10.293	-35.772	-41.793	1.00	37.73
BBBBATOM	5184	CD	ARG	B	345	11.716	-35.880	-41.284	1.00	40.70
BBBBATOM	5185	NE	ARG	B	345	12.580	-34.864	-41.873	1.00	44.36
BBBBATOM	5186	CZ	ARG	B	345	13.901	-34.841	-41.739	1.00	45.65
BBBBATOM	5187	NH1	ARG	B	345	14.514	-35.782	-41.031	1.00	46.05
BBBBATOM	5188	NH2	ARG	B	345	14.608	-33.881	-42.322	1.00	47.38
BBBBATOM	5189	C	ARG	B	345	7.626	-38.545	-41.854	1.00	30.89
BBBBATOM	5190	O	ARG	B	345	7.724	-39.387	-42.746	1.00	29.98
BBBBATOM	5191	N	VAL	B	346	7.086	-38.818	-40.670	1.00	29.72
BBBBATOM	5192	CA	VAL	B	346	6.578	-40.151	-40.384	1.00	28.61
BBBBATOM	5193	CB	VAL	B	346	6.197	-40.298	-38.885	1.00	27.90
BBBBATOM	5194	CG1	VAL	B	346	5.612	-41.680	-38.625	1.00	27.30
BBBBATOM	5195	CG2	VAL	B	346	7.419	-40.060	-38.024	1.00	27.32
BBBBATOM	5196	C	VAL	B	346	5.361	-40.435	-41.252	1.00	28.33
BBBBATOM	5197	O	VAL	B	346	5.248	-41.511	-41.847	1.00	28.30
BBBBATOM	5198	N	ALA	B	347	4.457	-39.465	-41.335	1.00	28.76
BBBBATOM	5199	CA	ALA	B	347	3.249	-39.617	-42.137	1.00	28.96
BBBBATOM	5200	CB	ALA	B	347	2.363	-38.387	-41.994	1.00	28.49
BBBBATOM	5201	C	ALA	B	347	3.596	-39.844	-43.606	1.00	30.26
BBBBATOM	5202	O	ALA	B	347	2.948	-40.641	-44.279	1.00	30.12
BBBBATOM	5203	N	ASN	B	348	4.613	-39.142	-44.098	1.00	32.77
BBBBATOM	5204	CA	ASN	B	348	5.035	-39.286	-45.493	1.00	34.56
BBBBATOM	5205	CB	ASN	B	348	6.045	-38.195	-45.868	1.00	35.68
BBBBATOM	5206	CG	ASN	B	348	5.384	-36.846	-46.123	1.00	37.21
BBBBATOM	5207	OD1	ASN	B	348	4.157	-36.719	-46.081	1.00	38.48
BBBBATOM	5208	ND2	ASN	B	348	6.199	-35.831	-46.393	1.00	38.38
BBBBATOM	5209	C	ASN	B	348	5.633	-40.668	-45.765	1.00	34.90
BBBBATOM	5210	O	ASN	B	348	5.433	-41.233	-46.841	1.00	34.59
BBBBATOM	5211	N	GLU	B	349	6.366	-41.212	-44.794	1.00	35.20
BBBBATOM	5212	CA	GLU	B	349	6.954	-42.540	-44.956	1.00	34.86
BBBBATOM	5213	CB	GLU	B	349	8.004	-42.814	-43.879	1.00	34.59
BBBBATOM	5214	CG	GLU	B	349	9.404	-42.385	-44.259	1.00	38.16
BBBBATOM	5215	CD	GLU	B	349	9.865	-42.992	-45.579	1.00	38.74
BBBBATOM	5216	OE1	GLU	B	349	9.806	-44.232	-45.735	1.00	40.12
BBBBATOM	5217	OE2	GLU	B	349	10.292	-42.225	-46.461	1.00	39.64
BBBBATOM	5218	C	GLU	B	349	5.872	-43.607	-44.895	1.00	33.96
BBBBATOM	5219	O	GLU	B	349	5.942	-44.621	-45.591	1.00	33.99
BBBBATOM	5220	N	VAL	B	350	4.875	-43.377	-44.051	1.00	33.91
BBBBATOM	5221	CA	VAL	B	350	3.767	-44.306	-43.919	1.00	33.79
BBBBATOM	5222	CB	VAL	B	350	2.848	-43.907	-42.744	1.00	33.70
BBBBATOM	5223	CG1	VAL	B	350	1.554	-44.695	-42.798	1.00	32.22
BBBBATOM	5224	CG2	VAL	B	350	3.568	-44.154	-41.425	1.00	32.24
BBBBATOM	5225	C	VAL	B	350	2.969	-44.274	-45.217	1.00	34.78
BBBBATOM	5226	O	VAL	B	350	2.411	-45.285	-45.645	1.00	34.85
BBBBATOM	5227	N	SER	B	351	2.925	-43.102	-45.844	1.00	35.34
BBBBATOM	5228	CA	SER	B	351	2.196	-42.946	-47.095	1.00	36.67
BBBBATOM	5229	CB	SER	B	351	2.024	-41.462	-47.425	1.00	37.32
BBBBATOM	5230	OG	SER	B	351	1.241	-41.292	-48.590	1.00	37.74
BBBBATOM	5231	C	SER	B	351	2.958	-43.639	-48.222	1.00	37.35
BBBBATOM	5232	O	SER	B	351	2.365	-44.309	-49.064	1.00	36.85
BBBBATOM	5233	N	ARG	B	352	4.277	-43.482	-48.223	1.00	37.89
BBBBATOM	5234	CA	ARG	B	352	5.114	-44.088	-49.251	1.00	40.03
BBBBATOM	5235	CB	ARG	B	352	6.557	-43.600	-49.114	1.00	41.58
BBBBATOM	5236	CG	ARG	B	352	7.470	-44.069	-50.232	1.00	44.46
BBBBATOM	5237	CD	ARG	B	352	8.906	-44.157	-49.759	1.00	47.36
BBBBATOM	5238	NE	ARG	B	352	9.097	-45.271	-48.832	1.00	49.57
BBBBATOM	5239	CZ	ARG	B	352	10.234	-45.524	-48.191	1.00	50.54
BBBBATOM	5240	*NH1	ARG	B	352	11.287	-44.738	-48.372	1.00	50.88

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BBBBATOM    5241  NH2 ARG B 352      10.321 -46.566 -47.373  1.00 50.24
BBBBATOM    5242  C   ARG B 352       5.098 -45.613 -49.176  1.00 40.60
BBBBATOM    5243  O   ARG B 352       5.101 -46.292 -50.204  1.00 39.84
BBBBATOM    5244  N   VAL B 353       5.096 -46.143 -47.955  1.00 41.33
BBBBATOM    5245  CA  VAL B 353       5.089 -47.587 -47.737  1.00 42.78
BBBBATOM    5246  CB  VAL B 353       5.446 -47.927 -46.271  1.00 42.54
BBBBATOM    5247  CG1 VAL B 353       5.279 -49.420 -46.014  1.00 42.05
BBBBATOM    5248  CG2 VAL B 353       6.879 -47.509 -45.987  1.00 41.86
BBBBATOM    5249  C   VAL B 353       3.742 -48.206 -48.095  1.00 43.85
BBBBATOM    5250  O   VAL B 353       3.679 -49.343 -48.556  1.00 44.43
BBBBATOM    5251  N   ALA B 354       2.664 -47.465 -47.871  1.00 45.85
BBBBATOM    5252  CA  ALA B 354       1.336 -47.957 -48.212  1.00 47.24
BBBBATOM    5253  CB  ALA B 354       0.264 -47.043 -47.628  1.00 46.79
BBBBATOM    5254  C   ALA B 354       1.250 -47.971 -49.737  1.00 48.54
BBBBATOM    5255  O   ALA B 354       0.531 -48.780 -50.324  1.00 48.48
BBBBATOM    5256  N   ARG B 355       1.998 -47.068 -50.366  1.00 50.49
BBBBATOM    5257  CA  ARG B 355       2.035 -46.964 -51.824  1.00 52.71
BBBBATOM    5258  CB  ARG B 355       2.658 -45.633 -52.264  1.00 53.58
BBBBATOM    5259  CG  ARG B 355       1.998 -44.372 -51.730  1.00 55.08
BBBBATOM    5260  CD  ARG B 355       0.716 -44.014 -52.461  1.00 56.64
BBBBATOM    5261  NE  ARG B 355       0.112 -42.802 -51.907  1.00 57.43
BBBBATOM    5262  CZ  ARG B 355      -1.054 -42.296 -52.299  1.00 58.24
BBBBATOM    5263  NH1 ARG B 355      -1.758 -42.896 -53.252  1.00 58.53
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BBBBATOM    5265  C   ARG B 355       2.899 -48.099 -52.366  1.00 53.41
BBBBATOM    5266  O   ARG B 355       2.966 -48.319 -53.575  1.00 53.50
BBBBATOM    5267  N   ALA B 356       3.569 -48.805 -51.456  1.00 54.15
BBBBATOM    5268  CA  ALA B 356       4.453 -49.913 -51.809  1.00 54.93
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BBBBATOM    5270  C   ALA B 356       5.611 -49.417 -52.671  1.00 55.63
BBBBATOM    5271  O   ALA B 356       6.193 -50.178 -53.442  1.00 55.95
BBBBATOM    5272  N   LEU B 357       5.942 -48.136 -52.526  1.00 56.45
BBBBATOM    5273  CA  LEU B 357       7.023 -47.522 -53.289  1.00 57.81
BBBBATOM    5274  CB  LEU B 357       6.871 -45.997 -53.290  1.00 58.04
BBBBATOM    5275  CG  LEU B 357       5.595 -45.422 -53.915  1.00 58.29
BBBBATOM    5276  CD1 LEU B 357       5.624 -43.903 -53.820  1.00 58.36
BBBBATOM    5277  CD2 LEU B 357       5.485 -45.859 -55.370  1.00 58.62
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BBBBATOM    5279  OT1 LEU B 357       9.244 -48.359 -53.514  1.00 58.97
BBBBATOM    5280  OT2 LEU B 357       8.601 -47.710 -51.512  1.00 58.97
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WATR
ATOM    5283  OH2 WAT W   5      20.119 -17.520 -22.473  1.00 21.13
WATR
ATOM    5284  OH2 WAT W   6      18.858 -19.701 -23.468  1.00 18.31
WATR
ATOM    5285  OH2 WAT W   7       2.329 -28.724 -15.978  1.00 27.32
WATR
ATOM    5286  OH2 WAT W   8       9.484 -48.435 -27.938  1.00 23.67
WATR
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WATR
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WATR
ATOM    5289  OH2 WAT W  11       5.875 -50.793 -32.396  1.00 20.21
WATR
ATOM    5290  OH2 WAT W  12      27.592 -18.174 -27.779  1.00 22.52
WATR
ATOM    5291  OH2 WAT W  13       7.842 -13.432 -21.178  1.00 25.85
WATR
ATOM    5292  OH2 WAT W  14       4.845 -57.924 -27.444  1.00 24.35
WATR
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ATOM   5293  OH2 WAT W  15       0.473 -58.751 -17.746  1.00 35.49
WATR
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WATR
ATOM   5295  OH2 WAT W  17      -8.656  11.300  18.872  1.00 23.81
WATR
ATOM   5296  OH2 WAT W  18       8.711 -45.913 -29.121  1.00 21.55
WATR
ATOM   5297  OH2 WAT W  19       2.957 -68.158 -38.242  1.00 29.43
WATR
ATOM   5298  OH2 WAT W  20      16.486 -11.742 -16.567  1.00 22.13
WATR
ATOM   5299  OH2 WAT W  21      -6.251  17.702  28.534  1.00 24.24
WATR
ATOM   5300  OH2 WAT W  22      12.670 -47.636 -24.808  1.00 25.87
WATR
ATOM   5301  OH2 WAT W  23       6.513 -15.597 -22.517  1.00 26.31
WATR
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WATR
ATOM   5303  OH2 WAT W  25     -29.060  13.621  26.406  1.00 21.08
WATR
ATOM   5304  OH2 WAT W  26      -5.240  10.154  13.527  1.00 29.62
WATR
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WATR
ATOM   5306  OH2 WAT W  28      18.996 -28.763 -24.427  1.00 20.28
WATR
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WATR
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ATOM   5314  OH2 WAT W  36       0.540  14.225  10.932  1.00 26.89
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WATR
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WATR
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WATR
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WATR
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WATR
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WATR
ATOM   5322  OH2 WAT W  44       7.131  -6.595 -18.003  1.00 29.47
WATR
ATOM   5323  OH2 WAT W  45      30.256 -23.202 -11.163  1.00 33.81
WATR
ATOM   5324  OH2 WAT W  46      -6.107 -66.004 -38.690  1.00 30.45
WATR
ATOM   5325  OH2 WAT W  47      17.631 -17.241  -5.864  1.00 28.69
WATR
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WATR
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WATR
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WATR
ATOM   5330  OH2 WAT W  52       9.140  -8.260 -23.371  1.00 40.29
WATR
ATOM   5331  OH2 WAT W  53     -19.061  14.438  38.966  1.00 38.01
WATR
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WATR
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WATR
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WATR
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WATR
ATOM   5340  OH2 WAT W  62      -9.797  12.718  13.997  1.00 29.14
WATR
ATOM   5341  OH2 WAT W  63      16.793   0.356  -6.115  1.00 26.17
WATR
ATOM   5342  OH2 WAT W  64       3.173  18.778  20.793  1.00 31.13
WATR
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WATR
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WATR
ATOM   5345  OH2 WAT W  67     -22.179   3.583  26.978  1.00 32.28
WATR
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WATR
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WATR
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WATR
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WATR
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WATR
ATOM   5352  OH2 WAT W  74      21.404 -42.041 -26.621  1.00 31.41
WATRATOM   5353  OH2 WAT W  75      -1.110 -15.319  -1.089  1.00 31.51
WATRATOM   5354  OH2 WAT W  76       0.688  19.730  22.519  1.00 26.71
WATRATOM   5355  OH2 WAT W  77      12.113 -69.335 -26.593  1.00 27.11
WATRATOM   5356  OH2 WAT W  78      11.725 -25.065 -33.817  1.00 43.79
WATRATOM   5357  OH2 WAT W  79     -25.519   9.450  22.092  1.00 28.18
WATRATOM   5358  OH2 WAT W  80     -14.673   6.584  16.023  1.00 31.37
WATRATOM   5359  OH2 WAT W  81      -2.250  -0.253  -1.741  1.00 29.99
WATRATOM   5360  OH2 WAT W  82      -7.300  12.943   8.415  1.00 32.39
WATRATOM   5361  OH2 WAT W  83       1.712 -13.629 -13.904  1.00 34.08
WATRATOM   5362  OH2 WAT W  84       4.709 -17.478  -6.557  1.00 29.67
WATRATOM   5363  OH2 WAT W  85      10.070 -57.496 -44.450  1.00 48.39
WATRATOM   5364  OH2 WAT W  86       8.040 -30.281 -10.117  1.00 28.59
WATRATOM   5365  OH2 WAT W  87      -1.967 -32.372 -38.643  1.00 31.55
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WATRATOM   5366  OH2 WAT W  88     -3.178 -64.576 -25.506  1.00 33.66
WATRATOM   5367  OH2 WAT W  89     15.762  -9.860 -10.400  1.00 34.29
WATRATOM   5368  OH2 WAT W  90      5.654 -30.990 -27.758  1.00 35.84
WATRATOM   5369  OH2 WAT W  91     14.959 -46.096 -42.270  1.00 35.21
WATRATOM   5370  OH2 WAT W  92     10.137 -13.308  -9.753  1.00 32.65
WATRATOM   5371  OH2 WAT W  93     -4.480   6.624   6.614  1.00 27.37
WATRATOM   5372  OH2 WAT W  94    -14.574  22.522  18.870  1.00 49.48
WATRATOM   5373  OH2 WAT W  95    -11.031 -42.768 -39.637  1.00 37.63
WATRATOM   5374  OH2 WAT W  96      9.906 -35.479 -19.203  1.00 29.59
WATRATOM   5375  OH2 WAT W  97     -0.990  -0.781  36.951  1.00 37.27
WATRATOM   5376  OH2 WAT W  98    -11.422   9.059  11.252  1.00 30.43
WATRATOM   5377  OH2 WAT W  99      8.118 -36.710 -22.371  1.00 34.85
WATRATOM   5378  OH2 WAT W 100     12.414 -67.326 -22.791  1.00 31.24
WATRATOM   5379  OH2 WAT W 101     28.541 -24.603 -31.049  1.00 40.14
WATRATOM   5380  OH2 WAT W 102     16.276 -10.934  -3.673  1.00 33.80
WATRATOM   5381  OH2 WAT W 103     30.979 -13.264 -22.953  1.00 24.73
WATRATOM   5382  OH2 WAT W 104     12.759 -31.636 -31.838  1.00 26.40
WATRATOM   5383  OH2 WAT W 105     23.507 -29.661 -32.187  1.00 29.62
WATRATOM   5384  OH2 WAT W 106     21.292 -13.141 -24.874  1.00 37.83
WATRATOM   5385  OH2 WAT W 107     10.171 -32.960 -15.580  1.00 26.59
WATRATOM   5386  OH2 WAT W 108     -2.207   2.376   2.034  1.00 27.55
WATRATOM   5387  OH2 WAT W 109     -6.984  22.588  16.082  1.00 39.01
WATRATOM   5388  OH2 WAT W 110     14.308 -11.038 -15.406  1.00 26.48
WATRATOM   5389  OH2 WAT W 111     10.612   9.749  24.161  1.00 40.18
WATRATOM   5390  OH2 WAT W 112      2.406 -15.823 -10.196  1.00 27.61
WATRATOM   5391  OH2 WAT W 113      6.310 -68.984 -20.661  1.00 40.25
WATRATOM   5392  OH2 WAT W 114     14.379 -10.930  -8.565  1.00 35.86
WATRATOM   5393  OH2 WAT W 115     24.183 -35.475 -30.338  1.00 35.17
WATRATOM   5394  OH2 WAT W 116     21.897 -31.717  -1.243  1.00 47.61
WATRATOM   5395  OH2 WAT W 117     24.065 -17.545 -13.707  1.00 32.24
WATRATOM   5396  OH2 WAT W 118     16.772 -51.926 -25.940  1.00 38.66
WATRATOM   5397  OH2 WAT W 119     -5.862   6.629   4.446  1.00 39.57
WATRATOM   5398  OH2 WAT W 120     14.133 -57.303 -28.159  1.00 30.19
WATRATOM   5399  OH2 WAT W 121    -16.538  -6.724  21.638  1.00 40.50
WATRATOM   5400  OH2 WAT W 122     19.669 -18.487 -33.216  1.00 38.38
WATRATOM   5401  OH2 WAT W 123     15.481   1.078  -4.048  1.00 32.28
WATRATOM   5402  OH2 WAT W 124     20.395 -13.033  -2.072  1.00 49.69
WATRATOM   5403  OH2 WAT W 125     15.526  -1.437 -15.842  1.00 36.06
WATRATOM   5404  OH2 WAT W 126      7.297 -29.419  -1.509  1.00 34.75
WATRATOM   5405  OH2 WAT W 127      9.994 -12.069 -21.013  1.00 32.21
WATRATOM   5406  OH2 WAT W 128     17.433 -42.825 -16.713  1.00 31.02
WATRATOM   5407  OH2 WAT W 129    -15.855  20.882  21.019  1.00 44.11
WATRATOM   5408  OH2 WAT W 130     -6.351  -7.687 -14.067  1.00 35.04
WATRATOM   5409  OH2 WAT W 131      7.954 -17.872  -1.475  1.00 28.45
WATRATOM   5410  OH2 WAT W 132     13.526 -34.593 -31.844  1.00 31.12
WATRATOM   5411  OH2 WAT W 133      9.992 -41.228 -23.098  1.00 26.45
WATRATOM   5412  OH2 WAT W 134      8.434  18.132  16.019  1.00 32.97
WATRATOM   5413  OH2 WAT W 135     -1.208 -33.658 -36.216  1.00 38.33
WATRATOM   5414  OH2 WAT W 136    -14.502   9.100  12.433  1.00 43.21
WATRATOM   5415  OH2 WAT W 137     14.394 -43.675 -17.325  1.00 32.32
WATRATOM   5416  OH2 WAT W 138     -4.809 -30.333 -46.416  1.00 42.65
WATRATOM   5417  OH2 WAT W 139     18.861 -35.072 -35.671  1.00 43.56
WATRATOM   5418  OH2 WAT W 140    -10.162 -60.139 -32.862  1.00 35.41
WATRATOM   5419  OH2 WAT W 141      6.740 -32.411 -35.303  1.00 38.57
WATRATOM   5420  OH2 WAT W 142    -12.257 -60.854 -39.307  1.00 32.90
WATRATOM   5421  OH2 WAT W 143     18.910 -40.984 -13.084  1.00 43.43
WATRATOM   5422  OH2 WAT W 144     18.857 -49.375 -28.645  1.00 31.34
WATRATOM   5423  OH2 WAT W 145      0.235 -17.424 -16.608  1.00 38.85
WATRATOM   5424  OH2 WAT W 146     14.236 -11.252 -24.086  1.00 27.79
WATRATOM   5425  OH2 WAT W 147     31.513 -22.336 -22.128  1.00 43.18
WATRATOM   5426  OH2 WAT W 148     -5.314 -70.396 -26.090  1.00 43.91
WATRATOM   5427  OH2 WAT W 149     -7.717 -64.969 -36.808  1.00 26.30
WATRATOM   5428  OH2 WAT W 150     22.584 -12.594  -4.179  1.00 46.91
WATRATOM   5429  OH2 WAT W 151    -12.388   9.493  36.619  1.00 32.82
WATRATOM   5430  OH2 WAT W 152    -14.517  16.479  37.760  1.00 39.52
WATRATOM   5431  OH2 WAT W 153    -10.095 -34.647 -29.068  1.00 41.08
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WATRATOM	5432	OH2	WAT	W	154	-5.233	-4.134	31.160	1.00	35.31
WATRATOM	5433	OH2	WAT	W	155	-6.322	11.278	-1.883	1.00	35.75
WATRATOM	5434	OH2	WAT	W	156	10.262	-9.572	-16.736	1.00	42.40
WATRATOM	5435	OH2	WAT	W	157	22.929	-10.414	-23.566	1.00	36.66
WATRATOM	5436	OH2	WAT	W	158	-15.987	3.994	16.559	1.00	37.22
WATRATOM	5437	OH2	WAT	W	159	13.385	-44.923	-46.826	1.00	41.55
WATRATOM	5438	OH2	WAT	W	160	26.508	-13.616	-18.049	1.00	25.93
WATRATOM	5439	OH2	WAT	W	161	4.671	-66.907	-17.861	1.00	31.54
WATRATOM	5440	OH2	WAT	W	162	-12.589	12.262	11.825	1.00	32.71
WATRATOM	5441	OH2	WAT	W	163	13.899	-62.269	-25.144	1.00	30.71
WATRATOM	5442	OH2	WAT	W	164	-31.053	15.663	19.272	1.00	30.19
WATRATOM	5443	OH2	WAT	W	165	9.797	-47.899	-25.140	1.00	26.79
WATRATOM	5444	OH2	WAT	W	166	0.877	-51.774	-25.619	1.00	30.02
WATRATOM	5445	OH2	WAT	W	167	-17.088	16.246	37.180	1.00	25.63
WATRATOM	5446	OH2	WAT	W	168	0.855	-52.086	-22.078	1.00	40.99
WATRATOM	5447	OH2	WAT	W	169	-14.873	18.295	21.203	1.00	40.28
WATRATOM	5448	OH2	WAT	W	170	11.913	-62.134	-35.641	1.00	41.33
WATRATOM	5449	OH2	WAT	W	171	25.783	-23.984	-33.162	1.00	44.03
WATRATOM	5450	OH2	WAT	W	172	7.169	-50.047	-23.737	1.00	47.85
WATRATOM	5451	OH2	WAT	W	173	20.074	-42.845	-14.939	1.00	32.87
WATRATOM	5452	OH2	WAT	W	174	8.765	5.909	9.193	1.00	34.30
WATRATOM	5453	OH2	WAT	W	175	-4.953	-64.494	-45.351	1.00	47.11
WATRATOM	5454	OH2	WAT	W	176	11.889	-61.263	-22.531	1.00	36.63
WATRATOM	5455	OH2	WAT	W	177	2.149	-49.169	-24.836	1.00	39.21
WATRATOM	5456	OH2	WAT	W	178	-14.051	6.399	13.353	1.00	39.89
WATRATOM	5457	OH2	WAT	W	179	8.488	-46.760	-23.118	1.00	45.24
WATRATOM	5458	OH2	WAT	W	180	-1.152	-23.348	-11.975	1.00	30.36
WATRATOM	5459	OH2	WAT	W	181	-7.002	3.531	7.051	1.00	44.50
WATRATOM	5460	OH2	WAT	W	182	-12.320	-54.772	-29.990	1.00	38.61
WATRATOM	5461	OH2	WAT	W	183	6.790	-54.559	-47.733	1.00	44.05
WATRATOM	5462	OH2	WAT	W	184	26.305	-38.240	-19.177	1.00	39.53
WATRATOM	5463	OH2	WAT	W	185	20.402	-58.179	-34.391	1.00	46.11
WATRATOM	5464	OH2	WAT	W	186	8.061	-31.341	-19.653	1.00	41.37
WATRATOM	5465	OH2	WAT	W	187	-7.549	-15.619	-5.482	1.00	40.60
WATRATOM	5466	OH2	WAT	W	188	-31.099	11.941	25.471	1.00	38.80
WATRATOM	5467	OH2	WAT	W	189	28.566	-25.441	-15.103	1.00	34.75
WATRATOM	5468	OH2	WAT	W	190	-5.613	-40.109	-50.158	1.00	49.21
WATRATOM	5469	OH2	WAT	W	191	17.024	-13.428	1.709	1.00	39.93
WATRATOM	5470	OH2	WAT	W	192	-22.114	10.176	37.673	1.00	32.53
WATRATOM	5471	OH2	WAT	W	193	10.204	-29.330	-20.066	1.00	27.24
WATRATOM	5472	OH2	WAT	W	194	27.893	-25.793	-21.862	1.00	38.97
WATRATOM	5473	OH2	WAT	W	195	-5.582	17.681	32.898	1.00	43.64
WATRATOM	5474	OH2	WAT	W	196	23.004	-45.224	-27.870	1.00	43.04
WATRATOM	5475	OH2	WAT	W	197	5.189	-58.857	-25.016	1.00	28.15
WATRATOM	5476	OH2	WAT	W	198	-7.740	-56.165	-24.052	1.00	35.98
WATRATOM	5477	OH2	WAT	W	199	-8.156	24.723	26.733	1.00	45.54
WATRATOM	5478	OH2	WAT	W	200	23.286	-32.333	-33.400	1.00	38.12
WATRATOM	5479	OH2	WAT	W	201	30.646	-14.180	-20.528	1.00	31.01
WATRATOM	5480	OH2	WAT	W	202	-8.238	-4.609	29.299	1.00	39.76
WATRATOM	5481	OH2	WAT	W	203	19.370	0.814	-7.532	1.00	35.83
WATRATOM	5482	OH2	WAT	W	204	0.885	-27.619	-1.442	1.00	47.04
WATRATOM	5483	OH2	WAT	W	205	16.084	-56.649	-26.382	1.00	45.97
WATRATOM	5484	OH2	WAT	W	206	-0.698	-19.360	-9.869	1.00	37.53
WATRATOM	5485	OH2	WAT	W	207	0.682	-14.985	-15.794	1.00	33.35
WATRATOM	5486	OH2	WAT	W	208	1.646	17.427	31.991	1.00	40.39
WATRATOM	5487	OH2	WAT	W	209	-21.611	1.533	20.359	1.00	31.04
WATRATOM	5488	OH2	WAT	W	210	-5.143	-55.137	-45.825	1.00	30.17
WATRATOM	5489	OH2	WAT	W	211	-9.645	13.045	37.660	1.00	42.93
WATRATOM	5490	OH2	WAT	W	212	22.096	-11.242	-30.224	1.00	48.12
WATRATOM	5491	OH2	WAT	W	213	-5.759	2.610	-15.984	1.00	41.67
WATRATOM	5492	OH2	WAT	W	214	-4.323	7.731	-7.331	1.00	37.92
WATRATOM	5493	OH2	WAT	W	215	-5.450	7.197	10.632	1.00	33.99
WATRATOM	5494	OH2	WAT	W	216	2.330	-32.635	-34.500	1.00	38.85
WATRATOM	5495	OH2	WAT	W	217	-26.827	16.219	13.451	1.00	38.12
WATRATOM	5496	OH2	WAT	W	218	10.887	-51.427	-23.191	1.00	39.81
WATRATOM	5497	OH2	WAT	W	219	-9.020	19.746	-3.698	1.00	46.58

WATRATOM	5498	OH2	WAT	W	220	9.054	6.622	-0.709	1.00	34.14
WATRATOM	5499	OH2	WAT	W	221	4.173	-7.985	-23.786	1.00	32.75
WATRATOM	5500	OH2	WAT	W	222	0.983	16.806	3.910	1.00	40.83
WATRATOM	5501	OH2	WAT	W	223	2.222	-16.848	-6.783	1.00	33.50
WATRATOM	5502	OH2	WAT	W	224	13.627	1.072	-15.114	1.00	37.51
WATRATOM	5503	OH2	WAT	W	225	12.533	-14.212	-9.007	1.00	38.40
WATRATOM	5504	OH2	WAT	W	226	1.404	-7.852	5.396	1.00	38.55
WATRATOM	5505	OH2	WAT	W	227	31.159	-24.354	-31.143	1.00	37.67
WATRATOM	5506	OH2	WAT	W	228	-13.047	-60.728	-42.282	1.00	42.18
WATRATOM	5507	OH2	WAT	W	229	8.956	-37.681	-16.765	1.00	41.45
WATRATOM	5508	OH2	WAT	W	230	28.749	-13.637	-16.860	1.00	42.34
WATRATOM	5509	OH2	WAT	W	231	-4.461	19.451	8.684	1.00	36.17
WATRATOM	5510	OH2	WAT	W	232	-9.785	-66.504	-35.701	1.00	44.07
WATRATOM	5511	OH2	WAT	W	233	10.673	-41.619	-20.678	1.00	36.58
WATRATOM	5512	OH2	WAT	W	234	-15.694	1.684	32.613	1.00	44.04
WATRATOM	5513	OH2	WAT	W	235	3.345	1.229	9.738	1.00	35.70
WATRATOM	5514	OH2	WAT	W	236	-6.256	-68.913	-30.401	1.00	36.72
WATRATOM	5515	OH2	WAT	W	237	28.344	-21.326	-30.399	1.00	36.45
WATRATOM	5516	OH2	WAT	W	238	2.876	-34.368	-17.344	1.00	42.48
WATRATOM	5517	OH2	WAT	W	239	15.355	-11.202	2.371	1.00	38.84
WATRATOM	5518	OH2	WAT	W	240	27.066	-22.336	-6.437	1.00	37.37
WATRATOM	5519	OH2	WAT	W	241	2.222	18.464	26.994	1.00	35.75
WATRATOM	5520	OH2	WAT	W	242	15.052	-9.829	-31.019	1.00	44.31
WATRATOM	5521	OH2	WAT	W	243	10.351	-67.649	-21.184	1.00	35.79
WATRATOM	5522	OH2	WAT	W	244	-13.173	14.269	38.605	1.00	41.50
WATRATOM	5523	OH2	WAT	W	245	-7.569	9.658	0.793	1.00	37.62
WATRATOM	5524	OH2	WAT	W	246	-2.167	-47.395	-19.605	1.00	45.90
WATRATOM	5525	OH2	WAT	W	247	7.166	2.400	15.830	1.00	42.90
WATRATOM	5526	OH2	WAT	W	248	-11.231	-10.901	-10.057	1.00	45.28
WATRATOM	5527	OH2	WAT	W	249	5.684	-16.094	-26.796	1.00	44.76
WATRATOM	5528	OH2	WAT	W	250	-4.745	3.667	-18.932	1.00	46.20
WATRATOM	5529	OH2	WAT	W	251	-0.505	-22.136	-9.079	1.00	42.89
WATRATOM	5530	OH2	WAT	W	252	16.668	-37.987	-7.767	1.00	35.76
WATRATOM	5531	OH2	WAT	W	253	2.454	-18.256	-26.130	1.00	43.33
WATRATOM	5532	OH2	WAT	W	254	-8.367	-39.960	-21.638	1.00	43.07
WATRATOM	5533	OH2	WAT	W	255	15.642	7.805	9.633	1.00	47.78
WATRATOM	5534	OH2	WAT	W	256	13.660	-24.331	1.932	1.00	42.50
WATRATOM	5535	OH2	WAT	W	257	11.567	-6.104	-23.359	1.00	37.10
WATRATOM	5536	OH2	WAT	W	258	18.941	-16.698	0.528	1.00	40.97
WATRATOM	5537	OH2	WAT	W	259	-11.441	-63.514	-39.126	1.00	43.17
WATRATOM	5538	OH2	WAT	W	260	28.664	-39.605	-22.853	1.00	42.65
WATRATOM	5539	OH2	WAT	W	261	6.795	-6.961	31.114	1.00	38.28
WATRATOM	5540	OH2	WAT	W	262	7.077	-14.349	-24.858	1.00	41.00
WATRATOM	5541	OH2	WAT	W	263	-2.259	-48.991	-29.099	1.00	34.96
WATRATOM	5542	OH2	WAT	W	264	21.812	-44.128	-35.641	1.00	44.51
WATRATOM	5543	OH2	WAT	W	265	-27.570	4.389	13.296	1.00	48.63
WATRATOM	5544	OH2	WAT	W	266	13.573	-27.185	0.220	1.00	43.56
WATRATOM	5545	OH2	WAT	W	267	16.549	8.451	-13.582	1.00	44.84
WATRATOM	5546	OH2	WAT	W	268	-9.142	9.107	36.872	1.00	37.66
WATRATOM	5547	OH2	WAT	W	269	5.648	-11.797	-24.893	1.00	45.79
WATRATOM	5548	OH2	WAT	W	270	3.619	-14.850	-23.652	1.00	34.09
WATRATOM	5549	OH2	WAT	W	271	-8.129	-11.098	-16.064	1.00	39.37
WATRATOM	5550	OH2	WAT	W	272	-17.342	8.563	9.979	1.00	46.38
WATRATOM	5551	OH2	WAT	W	273	8.798	-36.348	-46.119	1.00	37.71
WATRATOM	5552	OH2	WAT	W	274	9.190	-10.509	-35.865	1.00	45.80
WATRATOM	5553	OH2	WAT	W	275	13.545	-13.441	3.898	1.00	42.83
WATRATOM	5554	OH2	WAT	W	276	-7.844	0.944	-2.560	1.00	46.27
WATRATOM	5555	OH2	WAT	W	277	0.478	-47.721	-55.170	1.00	46.25
WATRATOM	5556	OH2	WAT	W	278	24.658	-18.359	-11.005	1.00	36.33
WATRATOM	5557	OH2	WAT	W	279	-4.675	21.561	12.155	1.00	37.17
WATRATOM	5558	OH2	WAT	W	280	0.382	20.486	4.930	1.00	41.40
WATRATOM	5559	OH2	WAT	W	281	5.919	18.010	25.033	1.00	41.72
WATRATOM	5560	OH2	WAT	W	282	-2.987	-63.751	-22.983	1.00	43.76
WATRATOM	5561	OH2	WAT	W	283	8.990	-33.134	-17.898	1.00	40.17
WATRATOM	5562	OH2	WAT	W	284	0.155	-61.872	-48.384	1.00	49.87
WATRATOM	5563	OH2	WAT	W	285	-10.443	-56.965	-24.681	1.00	48.02

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WATRATOM    5564  OH2 WAT W 286      18.915 -33.048  -3.930  1.00 37.81
WATRATOM    5565  OH2 WAT W 287     -16.181  11.706  12.277  1.00 41.77
WATRATOM    5566  OH2 WAT W 288       7.197   7.180  10.953  1.00 46.19
WATRATOM    5567  OH2 WAT W 289      31.934 -26.155 -26.053  1.00 38.77
WATRATOM    5568  OH2 WAT W 290     -15.232  -0.248  11.315  1.00 40.14
WATRATOM    5569  OH2 WAT W 291       9.450 -27.963  -1.396  1.00 41.29
WATRATOM    5570  OH2 WAT W 292      -1.800  13.139  -9.983  1.00 41.60
WATRATOM    5571  OH2 WAT W 293      -7.766   5.988   9.798  1.00 40.11
WATRATOM    5572  OH2 WAT W 294       7.973   4.338  14.321  1.00 39.97
WATRATOM    5573  OH2 WAT W 295      23.449 -40.563 -27.347  1.00 40.59
WATRATOM    5574  OH2 WAT W 296      -3.537 -28.260 -15.925  1.00 42.10
WATRATOM    5575  OH2 WAT W 297      28.052 -32.620 -12.168  1.00 48.03
WATRATOM    5576  OH2 WAT W 298      20.655 -43.315 -28.829  1.00 40.17
WATR
ATOM    5577  S   SO4 S   1        1.273 -70.953 -23.009  1.00 22.99
SO4
ATOM    5578  O1  SO4 S   1        1.720 -71.882 -24.053  1.00 21.18
SO4
ATOM    5579  O2  SO4 S   1        0.908 -69.659 -23.626  1.00 22.47
SO4
ATOM    5580  O3  SO4 S   1        2.337 -70.752 -22.018  1.00 23.88
SO4
ATOM    5581  O4  SO4 S   1        0.088 -71.522 -22.328  1.00 22.50
SO4
TEREND
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TABLE 2 ATOMIC COORDINATES OF E.COLI MURG C-ALPHA

BACKBONE ATOMS

ATOM	2649	CA	LYS	B	7	-6.512	-45.403	-47.519	1.00	45.28	BBBB
ATOM	2651	CA	ARG	B	8	-6.682	-47.303	-44.240	1.00	38.63	BBBB
ATOM	2662	CA	LEU	B	9	-4.094	-47.039	-41.477	1.00	30.88	BBBB
ATOM	2670	CA	MET	B	10	-4.048	-49.055	-38.275	1.00	26.66	BBBB
ATOM	2678	CA	VAL	B	11	-1.982	-47.605	-35.449	1.00	23.16	BBBB
ATOM	2685	CA	MET	B	12	-0.523	-49.707	-32.613	1.00	24.54	BBBB
ATOM	2693	CA	ALA	B	13	0.508	-47.410	-29.752	1.00	29.43	BBBB
ATOM	2698	CA	GLY	B	14	-0.513	-47.804	-26.120	1.00	33.82	BBBB
ATOM	2702	CA	GLY	B	15	-0.700	-45.047	-23.536	1.00	36.08	BBBB
ATOM	2706	CA	THR	B	16	1.920	-46.787	-21.421	1.00	38.51	BBBB
ATOM	2713	CA	GLY	B	17	5.367	-45.567	-22.392	1.00	36.57	BBBB
ATOM	2717	CA	GLY	B	18	3.631	-42.529	-23.872	1.00	33.48	BBBB
ATOM	2721	CA	HIS	B	19	3.548	-43.865	-27.435	1.00	28.22	BBBB
ATOM	2731	CA	VAL	B	20	-0.098	-42.894	-27.965	1.00	27.77	BBBB
ATOM	2738	CA	PHE	B	21	0.517	-39.136	-28.160	1.00	29.00	BBBB
ATOM	2750	CA	PRO	B	22	2.986	-39.252	-31.086	1.00	26.12	BBBB
ATOM	2756	CA	GLY	B	23	0.787	-41.864	-32.752	1.00	25.07	BBBB
ATOM	2760	CA	LEU	B	24	-2.201	-39.551	-32.401	1.00	25.32	BBBB
ATOM	2768	CA	ALA	B	25	-0.197	-36.754	-34.013	1.00	25.94	BBBB
ATOM	2773	CA	VAL	B	26	0.466	-38.955	-37.056	1.00	25.70	BBBB
ATOM	2780	CA	ALA	B	27	-3.116	-40.222	-37.199	1.00	26.15	BBBB
ATOM	2785	CA	HIS	B	28	-4.574	-36.702	-37.190	1.00	29.32	BBBB
ATOM	2795	CA	HIS	B	29	-2.070	-35.623	-39.806	1.00	32.38	BBBB
ATOM	2805	CA	LEU	B	30	-3.136	-38.417	-42.162	1.00	32.00	BBBB
ATOM	2813	CA	MET	B	31	-6.849	-38.064	-41.424	1.00	34.91	BBBB
ATOM	2821	CA	ALA	B	32	-6.510	-34.511	-42.722	1.00	37.55	BBBB
ATOM	2826	CA	GLN	B	33	-5.182	-36.070	-45.938	1.00	38.24	BBBB
ATOM	2835	CA	GLY	B	34	-8.305	-38.169	-46.353	1.00	35.75	BBBB
ATOM	2839	CA	TRP	B	35	-7.016	-41.246	-44.508	1.00	34.58	BBBB
ATOM	2853	CA	GLN	B	36	-9.175	-43.535	-42.402	1.00	35.40	BBBB
ATOM	2862	CA	VAL	B	37	-7.417	-44.516	-39.184	1.00	34.16	BBBB
ATOM	2869	CA	ARG	B	38	-8.219	-47.286	-36.730	1.00	31.56	BBBB
ATOM	2880	CA	TRP	B	39	-6.456	-48.070	-33.471	1.00	27.41	BBBB
ATOM	2894	CA	LEU	B	40	-5.200	-51.364	-32.026	1.00	24.71	BBBB
ATOM	2902	CA	GLY	B	41	-4.691	-51.450	-28.257	1.00	23.47	BBBB
ATOM	2906	CA	THR	B	42	-5.787	-53.141	-25.027	1.00	29.84	BBBB
ATOM	2913	CA	ALA	B	43	-9.000	-52.595	-23.047	1.00	38.81	BBBB
ATOM	2918	CA	ASP	B	44	-7.455	-51.942	-19.632	1.00	44.47	BBBB
ATOM	2926	CA	ARG	B	45	-4.887	-49.367	-20.763	1.00	40.44	BBBB
ATOM	2937	CA	MET	B	46	-4.881	-45.581	-21.249	1.00	36.33	BBBB
ATOM	2945	CA	GLU	B	47	-5.458	-45.655	-25.029	1.00	31.79	BBBB
ATOM	2954	CA	ALA	B	48	-8.821	-47.344	-24.414	1.00	32.58	BBBB
ATOM	2959	CA	ASP	B	49	-10.143	-44.065	-23.009	1.00	35.60	BBBB
ATOM	2967	CA	LEU	B	50	-8.026	-41.484	-24.840	1.00	33.49	BBBB
ATOM	2975	CA	VAL	B	51	-8.299	-42.641	-28.449	1.00	32.68	BBBB
ATOM	2983	CA	PRO	B	52	-12.111	-42.601	-28.453	1.00	34.43	BBBB
ATOM	2989	CA	LYS	B	53	-11.998	-39.054	-27.064	1.00	36.73	BBBB
ATOM	2998	CA	HIS	B	54	-10.116	-38.212	-30.259	1.00	34.62	BBBB
ATOM	3008	CA	GLY	B	55	-12.938	-39.481	-32.447	1.00	35.34	BBBB
ATOM	3012	CA	ILE	B	56	-10.909	-42.517	-33.514	1.00	33.81	BBBB
ATOM	3020	CA	GLU	B	57	-12.228	-46.083	-33.467	1.00	34.16	BBBB
ATOM	3029	CA	ILE	B	58	-10.217	-48.658	-31.553	1.00	31.38	BBBB
ATOM	3037	CA	ASP	B	59	-10.039	-52.442	-31.720	1.00	31.09	BBBB
ATOM	3045	CA	PHE	B	60	-8.809	-54.410	-28.713	1.00	30.32	BBBB
ATOM	3056	CA	ILE	B	61	-6.832	-57.616	-28.269	1.00	28.55	BBBB
ATOM	3064	CA	ARG	B	62	-5.709	-59.416	-25.133	1.00	30.76	BBBB
ATOM	3075	CA	ILE	B	63	-2.036	-59.770	-24.231	1.00	31.38	BBBB
ATOM	3083	CA	SER	B	64	-2.356	-60.520	-20.505	1.00	37.51	BBBB
ATOM	3089	CA	GLY	B	65	0.679	-62.355	-19.199	1.00	37.13	BBBB
ATOM	3093	CA	LEU	B	66	2.591	-61.413	-22.355	1.00	33.17	BBBB
ATOM	3101	CA	ARG	B	67	3.671	-57.928	-21.277	1.00	30.90	BBBB

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ATOM   3112  CA  GLY B  68       7.380 -57.427 -20.685  1.00 26.79 BBBB
ATOM   3116  CA  LYS B  69       8.238 -60.465 -22.796  1.00 23.93 BBBB
ATOM   3125  CA  GLY B  70      10.755 -60.229 -25.636  1.00 22.26 BBBB
ATOM   3129  CA  ILE B  71      10.357 -62.386 -28.762  1.00 23.55 BBBB
ATOM   3137  CA  LYS B  72      12.038 -65.491 -27.343  1.00 24.92 BBBB
ATOM   3146  CA  ALA B  73       9.839 -65.306 -24.233  1.00 21.18 BBBB
ATOM   3151  CA  LEU B  74       6.745 -64.762 -26.387  1.00 19.36 BBBB
ATOM   3159  CA  ILE B  75       7.434 -67.768 -28.601  1.00 21.18 BBBB
ATOM   3167  CA  ALA B  76       7.996 -69.726 -25.374  1.00 21.72 BBBB
ATOM   3172  CA  ALA B  77       4.289 -69.121 -24.655  1.00 21.07 BBBB
ATOM   3178  CA  PRO B  78       2.772 -70.846 -27.771  1.00 20.95 BBBB
ATOM   3184  CA  LEU B  79      -0.896 -70.728 -26.783  1.00 21.32 BBBB
ATOM   3192  CA  ARG B  80      -0.980 -67.115 -25.637  1.00 21.30 BBBB
ATOM   3203  CA  ILE B  81       1.113 -65.621 -28.421  1.00 19.47 BBBB
ATOM   3211  CA  PHE B  82      -0.875 -67.582 -31.038  1.00 19.15 BBBB
ATOM   3222  CA  ASN B  83      -4.150 -66.332 -29.577  1.00 20.90 BBBB
ATOM   3230  CA  ALA B  84      -3.177 -62.647 -29.484  1.00 19.30 BBBB
ATOM   3235  CA  TRP B  85      -1.820 -63.111 -33.032  1.00 20.56 BBBB
ATOM   3249  CA  ARG B  86      -5.140 -64.660 -34.166  1.00 23.28 BBBB
ATOM   3260  CA  GLN B  87      -7.101 -61.802 -32.567  1.00 24.07 BBBB
ATOM   3269  CA  ALA B  88      -4.996 -59.183 -34.355  1.00 23.78 BBBB
ATOM   3274  CA  ARG B  89      -5.285 -61.111 -37.636  1.00 24.94 BBBB
ATOM   3285  CA  ALA B  90      -9.088 -61.151 -37.383  1.00 26.16 BBBB
ATOM   3290  CA  ILE B  91      -9.108 -57.400 -36.733  1.00 26.97 BBBB
ATOM   3298  CA  MET B  92      -6.872 -56.693 -39.717  1.00 29.03 BBBB
ATOM   3306  CA  LYS B  93      -8.735 -59.038 -42.050  1.00 33.20 BBBB
ATOM   3315  CA  ALA B  94     -11.943 -57.157 -41.183  1.00 33.62 BBBB
ATOM   3320  CA  TYR B  95     -10.504 -53.620 -41.224  1.00 33.83 BBBB
ATOM   3332  CA  LYS B  96      -8.104 -54.327 -44.122  1.00 33.85 BBBB
ATOM   3342  CA  PRO B  97      -5.490 -51.623 -43.419  1.00 31.82 BBBB
ATOM   3348  CA  ASP B  98      -3.049 -50.685 -46.188  1.00 29.78 BBBB
ATOM   3356  CA  VAL B  99      -0.296 -50.214 -43.660  1.00 26.75 BBBB
ATOM   3363  CA  VAL B 100       0.227 -50.613 -39.936  1.00 23.59 BBBB
ATOM   3370  CA  LEU B 101       2.214 -48.199 -37.797  1.00 21.59 BBBB
ATOM   3378  CA  GLY B 102       3.796 -49.357 -34.549  1.00 19.23 BBBB
ATOM   3382  CA  MET B 103       4.892 -46.597 -32.191  1.00 18.93 BBBB
ATOM   3390  CA  GLY B 104       6.275 -49.080 -29.686  1.00 21.89 BBBB
ATOM   3394  CA  GLY B 105       4.593 -50.905 -26.827  1.00 23.54 BBBB
ATOM   3398  CA  TYR B 106       3.818 -54.554 -26.159  1.00 22.37 BBBB
ATOM   3410  CA  VAL B 107       0.557 -54.694 -28.099  1.00 18.06 BBBB
ATOM   3417  CA  SER B 108       2.488 -53.892 -31.290  1.00 19.67 BBBB
ATOM   3423  CA  GLY B 109       4.251 -57.256 -31.023  1.00 20.03 BBBB
ATOM   3428  CA  PRO B 110       1.251 -59.478 -31.855  1.00 18.99 BBBB
ATOM   3434  CA  GLY B 111      -0.160 -56.702 -34.025  1.00 19.60 BBBB
ATOM   3438  CA  GLY B 112       3.014 -56.417 -36.074  1.00 19.97 BBBB
ATOM   3442  CA  LEU B 113       3.265 -60.184 -36.429  1.00 19.49 BBBB
ATOM   3450  CA  ALA B 114      -0.334 -60.292 -37.661  1.00 18.70 BBBB
ATOM   3455  CA  ALA B 115       0.167 -57.516 -40.229  1.00 21.84 BBBB
ATOM   3460  CA  TRP B 116       3.365 -59.126 -41.478  1.00 23.22 BBBB
ATOM   3474  CA  SER B 117       1.735 -62.573 -41.873  1.00 22.61 BBBB
ATOM   3480  CA  LEU B 118      -1.069 -60.957 -43.882  1.00 25.70 BBBB
ATOM   3488  CA  GLY B 119       1.354 -59.174 -46.192  1.00 27.80 BBBB
ATOM   3492  CA  ILE B 120       0.568 -55.744 -44.731  1.00 24.85 BBBB
ATOM   3501  CA  PRO B 121       3.625 -53.477 -44.591  1.00 22.63 BBBB
ATOM   3507  CA  VAL B 122       4.743 -52.594 -41.083  1.00 22.03 BBBB
ATOM   3514  CA  VAL B 123       6.200 -49.184 -40.310  1.00 20.82 BBBB
ATOM   3521  CA  LEU B 124       7.749 -48.485 -36.915  1.00 22.10 BBBB
ATOM   3529  CA  HIS B 125       8.814 -45.413 -34.981  1.00 21.42 BBBB
ATOM   3539  CA  GLU B 126      10.947 -45.452 -31.817  1.00 22.15 BBBB
ATOM   3548  CA  GLN B 127      10.682 -42.270 -29.735  1.00 22.81 BBBB
ATOM   3557  CA  ASN B 128      13.406 -43.097 -27.216  1.00 22.96 BBBB
ATOM   3565  CA  GLY B 129      17.203 -43.019 -27.294  1.00 25.36 BBBB
ATOM   3569  CA  ILE B 130      17.160 -46.716 -26.488  1.00 28.00 BBBB
ATOM   3577  CA  ALA B 131      14.978 -49.139 -28.461  1.00 25.88 BBBB
ATOM   3582  CA  GLY B 132      12.007 -50.532 -26.568  1.00 24.05 BBBB
ATOM   3586  CA  LEU B 133      11.903 -54.293 -26.020  1.00 24.54 BBBB
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ATOM	3594	CA	THR	B	134	9.202	-54.860	-28.639	1.00	21.22	BBBB
ATOM	3601	CA	ASN	B	135	10.407	-52.419	-31.324	1.00	20.50	BBBB
ATOM	3609	CA	LYS	B	136	13.886	-53.949	-31.144	1.00	22.79	BBBB
ATOM	3618	CA	TRP	B	137	12.753	-57.345	-32.424	1.00	22.06	BBBB
ATOM	3632	CA	LEU	B	138	9.744	-56.188	-34.431	1.00	23.15	BBBB
ATOM	3640	CA	ALA	B	139	12.128	-54.092	-36.542	1.00	25.29	BBBB
ATOM	3645	CA	LYS	B	140	13.279	-57.337	-38.182	1.00	28.05	BBBB
ATOM	3654	CA	ILE	B	141	9.963	-57.818	-40.016	1.00	26.09	BBBB
ATOM	3662	CA	ALA	B	142	9.331	-54.107	-40.498	1.00	25.03	BBBB
ATOM	3667	CA	THR	B	143	9.262	-52.595	-43.984	1.00	26.10	BBBB
ATOM	3674	CA	LYS	B	144	10.436	-49.238	-42.618	1.00	24.73	BBBB
ATOM	3683	CA	VAL	B	145	11.947	-48.311	-39.252	1.00	23.62	BBBB
ATOM	3690	CA	MET	B	146	12.338	-44.736	-37.993	1.00	23.15	BBBB
ATOM	3698	CA	GLN	B	147	13.762	-43.418	-34.712	1.00	25.05	BBBB
ATOM	3707	CA	ALA	B	148	13.559	-40.032	-33.009	1.00	26.88	BBBB
ATOM	3712	CA	PHE	B	149	17.239	-39.820	-32.098	1.00	29.39	BBBB
ATOM	3724	CA	PRO	B	150	20.310	-41.541	-33.535	1.00	31.87	BBBB
ATOM	3730	CA	GLY	B	151	21.629	-44.537	-31.595	1.00	32.62	BBBB
ATOM	3734	CA	ALA	B	152	18.447	-46.476	-30.753	1.00	32.71	BBBB
ATOM	3739	CA	PHE	B	153	18.925	-48.506	-33.937	1.00	34.83	BBBB
ATOM	3751	CA	PRO	B	154	22.158	-48.751	-35.993	1.00	38.97	BBBB
ATOM	3757	CA	ASN	B	155	20.765	-47.568	-39.346	1.00	41.08	BBBB
ATOM	3765	CA	ALA	B	156	17.170	-46.407	-38.843	1.00	37.55	BBBB
ATOM	3770	CA	GLU	B	157	16.367	-43.044	-40.460	1.00	34.40	BBBB
ATOM	3779	CA	VAL	B	158	16.337	-40.344	-37.764	1.00	31.16	BBBB
ATOM	3786	CA	VAL	B	159	13.155	-38.265	-37.889	1.00	28.10	BBBB
ATOM	3793	CA	GLY	B	160	12.724	-36.921	-34.355	1.00	26.93	BBBB
ATOM	3797	CA	ASN	B	161	9.456	-36.807	-32.375	1.00	25.27	BBBB
ATOM	3806	CA	PRO	B	162	6.315	-34.747	-33.004	1.00	26.14	BBBB
ATOM	3812	CA	VAL	B	163	6.456	-31.379	-31.216	1.00	27.75	BBBB
ATOM	3819	CA	ARG	B	164	3.667	-28.953	-30.246	1.00	32.36	BBBB
ATOM	3830	CA	THR	B	165	3.038	-26.307	-32.924	1.00	31.74	BBBB
ATOM	3837	CA	ASP	B	166	3.252	-23.404	-30.466	1.00	30.64	BBBB
ATOM	3845	CA	VAL	B	167	6.746	-24.503	-29.440	1.00	25.91	BBBB
ATOM	3852	CA	LEU	B	168	7.780	-25.002	-33.075	1.00	28.46	BBBB
ATOM	3860	CA	ALA	B	169	6.580	-21.455	-33.756	1.00	31.43	BBBB
ATOM	3865	CA	LEU	B	170	9.002	-19.905	-31.268	1.00	29.60	BBBB
ATOM	3874	CA	PRO	B	171	11.611	-17.457	-32.642	1.00	30.11	BBBB
ATOM	3880	CA	LEU	B	172	15.157	-18.780	-33.062	1.00	28.33	BBBB
ATOM	3889	CA	PRO	B	173	17.450	-18.550	-29.977	1.00	25.25	BBBB
ATOM	3895	CA	GLN	B	174	19.526	-15.527	-31.049	1.00	25.46	BBBB
ATOM	3904	CA	GLN	B	175	16.365	-13.525	-31.718	1.00	28.47	BBBB
ATOM	3913	CA	ARG	B	176	14.611	-14.635	-28.525	1.00	29.01	BBBB
ATOM	3924	CA	LEU	B	177	17.673	-13.970	-26.331	1.00	29.90	BBBB
ATOM	3932	CA	ALA	B	178	18.766	-10.776	-28.131	1.00	30.78	BBBB
ATOM	3937	CA	GLY	B	179	19.846	-7.993	-25.784	1.00	30.10	BBBB
ATOM	3941	CA	ARG	B	180	18.676	-9.965	-22.787	1.00	28.97	BBBB
ATOM	3952	CA	GLU	B	181	20.545	-9.027	-19.621	1.00	31.79	BBBB
ATOM	3961	CA	GLY	B	182	19.871	-9.586	-15.943	1.00	27.75	BBBB
ATOM	3966	CA	PRO	B	183	19.450	-12.832	-13.913	1.00	22.93	BBBB
ATOM	3972	CA	VAL	B	184	19.524	-16.146	-15.729	1.00	18.01	BBBB
ATOM	3979	CA	ARG	B	185	15.873	-17.216	-16.011	1.00	17.62	BBBB
ATOM	3990	CA	VAL	B	186	15.508	-20.771	-14.741	1.00	16.47	BBBB
ATOM	3997	CA	LEU	B	187	12.361	-22.710	-15.604	1.00	16.75	BBBB
ATOM	4005	CA	VAL	B	188	11.774	-25.775	-13.381	1.00	18.41	BBBB
ATOM	4012	CA	VAL	B	189	9.298	-28.234	-14.948	1.00	22.11	BBBB
ATOM	4019	CA	GLY	B	190	7.914	-31.188	-12.994	1.00	27.28	BBBB
ATOM	4023	CA	GLY	B	191	4.935	-32.163	-15.115	1.00	31.94	BBBB
ATOM	4027	CA	SER	B	192	1.313	-32.665	-14.064	1.00	35.91	BBBB
ATOM	4033	CA	GLN	B	193	2.292	-34.763	-11.033	1.00	38.53	BBBB
ATOM	4042	CA	GLY	B	194	5.398	-32.711	-10.350	1.00	35.02	BBBB
ATOM	4046	CA	ALA	B	195	8.977	-33.819	-9.709	1.00	33.12	BBBB
ATOM	4051	CA	ARG	B	196	9.538	-34.512	-6.010	1.00	32.63	BBBB
ATOM	4062	CA	ILE	B	197	13.329	-34.168	-6.164	1.00	28.10	BBBB
ATOM	4070	CA	LEU	B	198	13.069	-30.833	-8.003	1.00	26.58	BBBB
ATOM	4078	CA	ASN	B	199	10.497	-29.447	-5.563	1.00	27.07	BBBB

ATOM	4086	CA	GLN	B	200	12.955	-30.326	-2.794	1.00	30.10	BBBB
ATOM	4095	CA	THR	B	201	16.215	-29.345	-4.474	1.00	27.34	BBBB
ATOM	4102	CA	MET	B	202	15.567	-26.048	-6.268	1.00	23.68	BBBB
ATOM	4111	CA	PRO	B	203	14.608	-23.963	-3.220	1.00	23.84	BBBB
ATOM	4117	CA	GLN	B	204	18.033	-24.708	-1.684	1.00	26.34	BBBB
ATOM	4126	CA	VAL	B	205	19.672	-24.033	-5.043	1.00	24.44	BBBB
ATOM	4133	CA	ALA	B	206	17.980	-20.610	-5.013	1.00	22.84	BBBB
ATOM	4138	CA	ALA	B	207	19.442	-19.857	-1.576	1.00	26.65	BBBB
ATOM	4143	CA	LYS	B	208	22.915	-20.595	-2.919	1.00	28.31	BBBB
ATOM	4152	CA	LEU	B	209	22.577	-18.640	-6.171	1.00	25.68	BBBB
ATOM	4160	CA	GLY	B	210	20.675	-15.628	-4.804	1.00	26.56	BBBB
ATOM	4164	CA	ASP	B	211	20.370	-12.647	-7.190	1.00	28.28	BBBB
ATOM	4172	CA	SER	B	212	22.098	-14.474	-10.067	1.00	25.73	BBBB
ATOM	4178	CA	VAL	B	213	18.925	-16.308	-11.116	1.00	20.76	BBBB
ATOM	4185	CA	THR	B	214	15.204	-15.726	-11.337	1.00	19.60	BBBB
ATOM	4192	CA	ILE	B	215	13.076	-18.850	-11.169	1.00	18.75	BBBB
ATOM	4200	CA	TRP	B	216	9.661	-19.973	-12.378	1.00	19.34	BBBB
ATOM	4214	CA	HIS	B	217	9.015	-23.303	-10.680	1.00	21.06	BBBB
ATOM	4224	CA	GLN	B	218	6.149	-25.594	-11.735	1.00	24.30	BBBB
ATOM	4233	CA	SER	B	219	5.463	-27.800	-8.684	1.00	26.73	BBBB
ATOM	4239	CA	GLY	B	220	2.855	-30.242	-9.961	1.00	30.53	BBBB
ATOM	4243	CA	LYS	B	221	-0.657	-30.914	-8.628	1.00	35.12	BBBB
ATOM	4252	CA	GLY	B	222	-1.195	-29.899	-5.011	1.00	35.34	BBBB
ATOM	4256	CA	SER	B	223	2.451	-28.934	-4.418	1.00	33.98	BBBB
ATOM	4262	CA	GLN	B	224	2.187	-25.208	-5.186	1.00	33.71	BBBB
ATOM	4271	CA	GLN	B	225	1.823	-24.239	-1.519	1.00	32.32	BBBB
ATOM	4280	CA	SER	B	226	4.701	-26.309	-0.122	1.00	28.30	BBBB
ATOM	4286	CA	VAL	B	227	7.214	-25.247	-2.791	1.00	24.28	BBBB
ATOM	4293	CA	GLU	B	228	6.178	-21.592	-2.387	1.00	27.23	BBBB
ATOM	4302	CA	GLN	B	229	6.853	-22.046	1.329	1.00	28.38	BBBB
ATOM	4311	CA	ALA	B	230	10.185	-23.754	0.682	1.00	26.18	BBBB
ATOM	4316	CA	TYR	B	231	11.371	-20.766	-1.366	1.00	25.47	BBBB
ATOM	4328	CA	ALA	B	232	10.342	-18.322	1.368	1.00	27.51	BBBB
ATOM	4333	CA	GLU	B	233	12.145	-20.441	3.966	1.00	30.87	BBBB
ATOM	4342	CA	ALA	B	234	15.215	-20.417	1.714	1.00	28.48	BBBB
ATOM	4347	CA	GLY	B	235	15.033	-16.627	1.815	1.00	26.23	BBBB
ATOM	4351	CA	GLN	B	236	14.121	-16.198	-1.870	1.00	25.53	BBBB
ATOM	4361	CA	PRO	B	237	10.336	-15.587	-1.720	1.00	24.65	BBBB
ATOM	4367	CA	GLN	B	238	10.277	-13.558	-4.945	1.00	24.29	BBBB
ATOM	4376	CA	HIS	B	239	10.526	-16.608	-7.201	1.00	22.08	BBBB
ATOM	4386	CA	LYS	B	240	7.375	-17.589	-9.105	1.00	23.26	BBBB
ATOM	4395	CA	VAL	B	241	5.740	-20.911	-8.277	1.00	23.78	BBBB
ATOM	4402	CA	THR	B	242	2.758	-22.301	-10.177	1.00	25.93	BBBB
ATOM	4409	CA	GLU	B	243	0.999	-25.651	-9.837	1.00	27.03	BBBB
ATOM	4418	CA	PHE	B	244	0.964	-26.068	-13.620	1.00	26.54	BBBB
ATOM	4429	CA	ILE	B	245	1.932	-24.242	-16.802	1.00	28.48	BBBB
ATOM	4437	CA	ASP	B	246	-0.754	-24.396	-19.457	1.00	36.00	BBBB
ATOM	4445	CA	ASP	B	247	1.245	-22.392	-21.999	1.00	30.74	BBBB
ATOM	4453	CA	MET	B	248	4.625	-24.136	-22.138	1.00	28.41	BBBB
ATOM	4461	CA	ALA	B	249	5.512	-22.216	-25.290	1.00	24.67	BBBB
ATOM	4466	CA	ALA	B	250	5.188	-18.933	-23.390	1.00	21.78	BBBB
ATOM	4471	CA	ALA	B	251	7.301	-20.259	-20.501	1.00	20.85	BBBB
ATOM	4476	CA	TYR	B	252	9.972	-21.616	-22.886	1.00	22.78	BBBB
ATOM	4488	CA	ALA	B	253	10.131	-18.224	-24.636	1.00	23.54	BBBB
ATOM	4493	CA	TRP	B	254	10.829	-16.534	-21.303	1.00	19.76	BBBB
ATOM	4507	CA	ALA	B	255	13.399	-19.025	-20.003	1.00	19.51	BBBB
ATOM	4512	CA	ASP	B	256	17.176	-19.026	-20.434	1.00	17.58	BBBB
ATOM	4520	CA	VAL	B	257	17.535	-22.603	-19.194	1.00	18.53	BBBB
ATOM	4527	CA	VAL	B	258	15.208	-25.456	-18.234	1.00	19.32	BBBB
ATOM	4534	CA	VAL	B	259	15.581	-27.957	-15.374	1.00	19.85	BBBB
ATOM	4541	CA	CYS	B	260	13.454	-31.055	-15.946	1.00	22.00	BBBB
ATOM	4547	CA	ARG	B	261	13.170	-34.800	-16.515	1.00	23.75	BBBB
ATOM	4558	CA	SER	B	262	13.975	-36.189	-19.948	1.00	23.18	BBBB
ATOM	4564	CA	GLY	B	263	11.026	-38.079	-21.361	1.00	22.85	BBBB
ATOM	4568	CA	ALA	B	264	11.482	-38.564	-25.115	1.00	24.25	BBBB
ATOM	4573	CA	LEU	B	265	8.846	-36.037	-26.205	1.00	24.66	BBBB

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ATOM   4581  CA  THR B 266      10.194 -33.557 -23.657  1.00 22.34 BBBB
ATOM   4588  CA  VAL B 267      13.730 -33.762 -25.023  1.00 21.11 BBBB
ATOM   4595  CA  SER B 268      12.411 -33.191 -28.567  1.00 21.96 BBBB
ATOM   4601  CA  GLU B 269      10.282 -30.272 -27.378  1.00 21.95 BBBB
ATOM   4610  CA  ILE B 270      13.295 -28.698 -25.638  1.00 20.62 BBBB
ATOM   4618  CA  ALA B 271      15.440 -29.058 -28.776  1.00 22.45 BBBB
ATOM   4623  CA  ALA B 272      12.719 -27.451 -30.898  1.00 22.17 BBBB
ATOM   4628  CA  ALA B 273      12.361 -24.596 -28.407  1.00 21.97 BBBB
ATOM   4633  CA  GLY B 274      16.093 -24.023 -28.709  1.00 21.07 BBBB
ATOM   4637  CA  LEU B 275      16.666 -24.057 -24.966  1.00 19.78 BBBB
ATOM   4646  CA  PRO B 276      19.651 -25.199 -22.875  1.00 16.62 BBBB
ATOM   4652  CA  ALA B 277      18.638 -27.807 -20.321  1.00 15.80 BBBB
ATOM   4657  CA  LEU B 278      19.896 -29.429 -17.145  1.00 18.48 BBBB
ATOM   4665  CA  PHE B 279      18.266 -32.838 -17.392  1.00 21.59 BBBB
ATOM   4676  CA  VAL B 280      17.502 -34.902 -14.281  1.00 25.67 BBBB
ATOM   4684  CA  PRO B 281      16.698 -38.320 -15.824  1.00 29.05 BBBB
ATOM   4690  CA  PHE B 282      14.246 -40.496 -13.926  1.00 37.13 BBBB
ATOM   4701  CA  GLN B 283      16.319 -43.395 -12.591  1.00 41.11 BBBB
ATOM   4710  CA  HIS B 284      15.641 -46.917 -13.843  1.00 43.69 BBBB
ATOM   4720  CA  LYS B 285      17.767 -49.993 -14.571  1.00 45.34 BBBB
ATOM   4729  CA  ASP B 286      16.949 -49.299 -18.222  1.00 43.26 BBBB
ATOM   4737  CA  ARG B 287      17.951 -45.623 -17.883  1.00 36.28 BBBB
ATOM   4748  CA  GLN B 288      15.622 -44.804 -20.755  1.00 30.77 BBBB
ATOM   4757  CA  GLN B 289      15.474 -41.099 -19.904  1.00 29.46 BBBB
ATOM   4766  CA  TYR B 290      19.228 -40.984 -19.550  1.00 29.55 BBBB
ATOM   4778  CA  TRP B 291      19.542 -42.282 -23.116  1.00 28.07 BBBB
ATOM   4792  CA  ASN B 292      16.902 -39.784 -24.270  1.00 26.06 BBBB
ATOM   4800  CA  ALA B 293      18.926 -36.822 -22.979  1.00 25.69 BBBB
ATOM   4805  CA  LEU B 294      22.354 -38.088 -24.032  1.00 25.90 BBBB
ATOM   4814  CA  PRO B 295      21.998 -36.870 -27.635  1.00 26.15 BBBB
ATOM   4820  CA  LEU B 296      21.521 -33.265 -26.481  1.00 25.42 BBBB
ATOM   4828  CA  GLU B 297      24.354 -33.530 -23.953  1.00 28.78 BBBB
ATOM   4837  CA  LYS B 298      26.644 -34.947 -26.648  1.00 31.90 BBBB
ATOM   4846  CA  ALA B 299      25.773 -31.965 -28.847  1.00 30.38 BBBB
ATOM   4851  CA  GLY B 300      26.777 -29.635 -26.017  1.00 26.18 BBBB
ATOM   4855  CA  ALA B 301      23.214 -28.333 -25.638  1.00 22.50 BBBB
ATOM   4860  CA  ALA B 302      22.516 -29.770 -22.186  1.00 21.78 BBBB
ATOM   4865  CA  LYS B 303      23.979 -31.340 -19.048  1.00 25.86 BBBB
ATOM   4874  CA  ILE B 304      22.753 -34.598 -17.550  1.00 27.17 BBBB
ATOM   4882  CA  ILE B 305      22.843 -35.178 -13.813  1.00 29.01 BBBB
ATOM   4890  CA  GLU B 306      21.664 -38.702 -13.061  1.00 34.65 BBBB
ATOM   4899  CA  GLN B 307      20.377 -39.599  -9.613  1.00 40.54 BBBB
ATOM   4909  CA  PRO B 308      23.828 -40.891  -8.484  1.00 43.20 BBBB
ATOM   4915  CA  GLN B 309      25.247 -37.361  -8.787  1.00 43.46 BBBB
ATOM   4924  CA  LEU B 310      22.232 -35.166  -8.022  1.00 39.65 BBBB
ATOM   4932  CA  SER B 311      22.660 -32.714  -5.154  1.00 34.90 BBBB
ATOM   4938  CA  VAL B 312      21.990 -29.074  -4.341  1.00 31.50 BBBB
ATOM   4945  CA  ASP B 313      25.642 -28.202  -4.957  1.00 29.61 BBBB
ATOM   4953  CA  ALA B 314      25.782 -30.099  -8.254  1.00 26.47 BBBB
ATOM   4958  CA  VAL B 315      22.755 -28.215  -9.612  1.00 25.33 BBBB
ATOM   4965  CA  ALA B 316      23.888 -24.872  -8.199  1.00 27.13 BBBB
ATOM   4970  CA  ASN B 317      27.444 -25.246  -9.518  1.00 28.52 BBBB
ATOM   4978  CA  THR B 318      26.174 -26.371 -12.906  1.00 27.04 BBBB
ATOM   4985  CA  LEU B 319      23.883 -23.370 -13.357  1.00 25.21 BBBB
ATOM   4993  CA  ALA B 320      26.445 -20.931 -11.957  1.00 24.59 BBBB
ATOM   4998  CA  GLY B 321      28.934 -22.031 -14.591  1.00 24.34 BBBB
ATOM   5002  CA  TRP B 322      26.738 -21.007 -17.521  1.00 21.72 BBBB
ATOM   5016  CA  SER B 323      27.141 -17.404 -18.692  1.00 19.04 BBBB
ATOM   5022  CA  ARG B 324      24.725 -15.741 -21.112  1.00 18.09 BBBB
ATOM   5033  CA  GLU B 325      27.220 -16.368 -23.954  1.00 16.96 BBBB
ATOM   5042  CA  THR B 326      27.460 -20.055 -23.070  1.00 16.39 BBBB
ATOM   5049  CA  LEU B 327      23.659 -20.305 -22.780  1.00 17.27 BBBB
ATOM   5057  CA  LEU B 328      23.175 -18.745 -26.222  1.00 17.39 BBBB
ATOM   5065  CA  THR B 329      25.567 -21.335 -27.688  1.00 21.30 BBBB
ATOM   5072  CA  MET B 330      23.771 -24.153 -25.870  1.00 19.91 BBBB
ATOM   5080  CA  ALA B 331      20.412 -22.871 -27.098  1.00 18.49 BBBB
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ATOM   5085  CA  GLU B 332      21.626 -22.827 -30.704  1.00 21.47  BBBB
ATOM   5094  CA  ARG B 333      23.040 -26.330 -30.408  1.00 23.77  BBBB
ATOM   5105  CA  ALA B 334      19.648 -27.420 -29.063  1.00 22.88  BBBB
ATOM   5110  CA  ARG B 335      17.795 -25.892 -32.002  1.00 23.54  BBBB
ATOM   5121  CA  ALA B 336      20.330 -27.477 -34.372  1.00 26.85  BBBB
ATOM   5126  CA  ALA B 337      19.740 -30.925 -32.865  1.00 30.89  BBBB
ATOM   5131  CA  SER B 338      16.008 -30.432 -33.408  1.00 32.41  BBBB
ATOM   5137  CA  ILE B 339      13.882 -31.941 -36.187  1.00 34.35  BBBB
ATOM   5146  CA  PRO B 340      10.733 -29.730 -36.600  1.00 34.94  BBBB
ATOM   5152  CA  ASP B 341       8.711 -31.820 -39.056  1.00 33.33  BBBB
ATOM   5160  CA  ALA B 342       8.875 -35.238 -37.411  1.00 29.09  BBBB
ATOM   5165  CA  THR B 343       5.115 -35.696 -37.744  1.00 28.55  BBBB
ATOM   5172  CA  GLU B 344       5.085 -34.933 -41.480  1.00 32.00  BBBB
ATOM   5181  CA  ARG B 345       8.138 -37.123 -42.067  1.00 31.44  BBBB
ATOM   5192  CA  VAL B 346       6.578 -40.151 -40.384  1.00 28.61  BBBB
ATOM   5199  CA  ALA B 347       3.249 -39.617 -42.137  1.00 28.96  BBBB
ATOM   5204  CA  ASN B 348       5.035 -39.286 -45.493  1.00 34.56  BBBB
ATOM   5212  CA  GLU B 349       6.954 -42.540 -44.956  1.00 34.86  BBBB
ATOM   5221  CA  VAL B 350       3.767 -44.306 -43.919  1.00 33.79  BBBB
ATOM   5228  CA  SER B 351       2.196 -42.946 -47.095  1.00 36.67  BBBB
ATOM   5234  CA  ARG B 352       5.114 -44.088 -49.251  1.00 40.03  BBBB
ATOM   5245  CA  VAL B 353       5.089 -47.587 -47.737  1.00 42.78  BBBB
ATOM   5252  CA  ALA B 354       1.336 -47.957 -48.212  1.00 47.24  BBBB
ATOM   5257  CA  ARG B 355       2.035 -46.964 -51.824  1.00 52.71  BBBB
ATOM   5268  CA  ALA B 356       4.453 -49.913 -51.809  1.00 54.93  BBBB
ATOM   5273  CA  LEU B 357       7.023 -47.522 -53.289  1.00 57.81  BBBB
END
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TABLE 3 ATOMIC COORDINATES OF E.COLI MURG C-ALPHA

BACKBONE AND CONSERVED AMINO ACID RESIDUES

ATOM	2649	CA	LYS	B	7	-6.512	-45.403	-47.519	1.00	45.28	BBBB
ATOM	2651	CA	ARG	B	8	-6.682	-47.303	-44.240	1.00	38.63	BBBB
ATOM	2662	CA	LEU	B	9	-4.094	-47.039	-41.477	1.00	30.88	BBBB
ATOM	2670	CA	MET	B	10	-4.048	-49.055	-38.275	1.00	26.66	BBBB
ATOM	2678	CA	VAL	B	11	-1.982	-47.605	-35.449	1.00	23.16	BBBB
ATOM	2685	CA	MET	B	12	-0.523	-49.707	-32.613	1.00	24.54	BBBB
ATOM	2693	CA	ALA	B	13	0.508	-47.410	-29.752	1.00	29.43	BBBB
ATOM	2697	N	GLY	B	14	0.150	-47.934	-27.405	1.00	32.46	BBBB
ATOM	2698	CA	GLY	B	14	-0.513	-47.804	-26.120	1.00	33.82	BBBB
ATOM	2699	C	GLY	B	14	-0.107	-46.595	-25.299	1.00	34.82	BBBB
ATOM	2700	O	GLY	B	14	0.975	-46.040	-25.479	1.00	35.47	BBBB
ATOM	2701	N	GLY	B	15	-0.986	-46.188	-24.385	1.00	35.56	BBBB
ATOM	2702	CA	GLY	B	15	-0.700	-45.047	-23.536	1.00	36.08	BBBB
ATOM	2703	C	GLY	B	15	0.539	-45.254	-22.683	1.00	36.84	BBBB
ATOM	2704	O	GLY	B	15	1.293	-44.311	-22.426	1.00	36.03	BBBB
ATOM	2706	CA	THR	B	16	1.920	-46.787	-21.421	1.00	38.51	BBBB
ATOM	2713	CA	GLY	B	17	5.367	-45.567	-22.392	1.00	36.57	BBBB
ATOM	2716	N	GLY	B	18	3.949	-43.752	-23.150	1.00	33.83	BBBB
ATOM	2717	CA	GLY	B	18	3.631	-42.529	-23.872	1.00	33.48	BBBB
ATOM	2718	C	GLY	B	18	3.825	-42.593	-25.378	1.00	33.12	BBBB
ATOM	2719	O	GLY	B	18	4.345	-41.650	-25.984	1.00	35.38	BBBB
ATOM	2720	N	HIS	B	19	3.416	-43.699	-25.988	1.00	30.26	BBBB
ATOM	2721	CA	HIS	B	19	3.548	-43.865	-27.435	1.00	28.22	BBBB
ATOM	2722	CB	HIS	B	19	3.772	-45.349	-27.779	1.00	25.81	BBBB
ATOM	2723	CG	HIS	B	19	4.957	-45.966	-27.094	1.00	25.35	BBBB
ATOM	2724	CD2	HIS	B	19	6.281	-45.694	-27.184	1.00	24.18	BBBB
ATOM	2725	ND1	HIS	B	19	4.845	-47.025	-26.217	1.00	24.57	BBBB
ATOM	2726	CE1	HIS	B	19	6.046	-47.380	-25.798	1.00	23.08	BBBB
ATOM	2727	NE2	HIS	B	19	6.936	-46.589	-26.369	1.00	25.51	BBBB
ATOM	2728	C	HIS	B	19	2.280	-43.370	-28.144	1.00	27.91	BBBB
ATOM	2729	O	HIS	B	19	2.300	-43.049	-29.337	1.00	26.91	BBBB
ATOM	2731	CA	VAL	B	20	-0.098	-42.894	-27.965	1.00	27.77	BBBB
ATOM	2738	CA	PHE	B	21	0.517	-39.136	-28.160	1.00	29.00	BBBB
ATOM	2750	CA	PRO	B	22	1.986	-39.252	-31.086	1.00	26.12	BBBB
ATOM	2756	CA	GLY	B	23	0.787	-41.864	-32.752	1.00	25.07	BBBB
ATOM	2760	CA	LEU	B	24	-2.201	-39.551	-32.401	1.00	25.32	BBBB
ATOM	2768	CA	ALA	B	25	-0.197	-36.754	-34.013	1.00	25.94	BBBB
ATOM	2773	CA	VAL	B	26	0.466	-38.955	-37.056	1.00	25.70	BBBB
ATOM	2780	CA	ALA	B	27	-3.116	-40.222	-37.199	1.00	26.15	BBBB
ATOM	2785	CA	HIS	B	28	-4.574	-36.702	-37.190	1.00	29.32	BBBB
ATOM	2795	CA	HIS	B	29	-2.070	-35.623	-39.806	1.00	32.38	BBBB
ATOM	2805	CA	LEU	B	30	-3.136	-38.417	-42.162	1.00	32.00	BBBB
ATOM	2813	CA	MET	B	31	-6.849	-38.064	-41.424	1.00	34.91	BBBB
ATOM	2821	CA	ALA	B	32	-6.510	-34.511	-42.722	1.00	37.55	BBBB
ATOM	2826	CA	GLN	B	33	-5.182	-36.070	-45.938	1.00	38.24	BBBB
ATOM	2835	CA	GLY	B	34	-8.305	-38.169	-46.353	1.00	35.75	BBBB
ATOM	2839	CA	TRP	B	35	-7.016	-41.246	-44.508	1.00	34.58	BBBB
ATOM	2853	CA	GLN	B	36	-9.175	-43.535	-42.402	1.00	35.40	BBBB
ATOM	2862	CA	VAL	B	37	-7.417	-44.516	-39.184	1.00	34.16	BBBB
ATOM	2869	CA	ARG	B	38	-8.219	-47.286	-36.730	1.00	31.56	BBBB
ATOM	2880	CA	TRP	B	39	-6.456	-48.070	-33.471	1.00	27.41	BBBB
ATOM	2894	CA	LEU	B	40	-5.200	-51.364	-32.026	1.00	24.71	BBBB
ATOM	2902	CA	GLY	B	41	-4.691	-51.450	-28.257	1.00	23.47	BBBB
ATOM	2906	CA	THR	B	42	-5.787	-53.141	-25.027	1.00	29.84	BBBB
ATOM	2913	CA	ALA	B	43	-9.000	-52.595	-23.047	1.00	38.81	BBBB
ATOM	2918	CA	ASP	B	44	-7.455	-51.942	-19.632	1.00	44.47	BBBB
ATOM	2926	CA	ARG	B	45	-4.887	-49.367	-20.763	1.00	40.44	BBBB
ATOM	2937	CA	MET	B	46	-4.881	-45.581	-21.249	1.00	36.33	BBBB
ATOM	2945	CA	GLU	B	47	-5.458	-45.655	-25.029	1.00	31.79	BBBB
ATOM	2954	CA	ALA	B	48	-8.821	-47.344	-24.414	1.00	32.58	BBBB
ATOM	2959	CA	ASP	B	49	-10.143	-44.065	-23.009	1.00	35.60	BBBB

ATOM	2967	CA	LEU	B	50	-8.026	-41.484	-24.840	1.00	33.49	BBBB
ATOM	2975	CA	VAL	B	51	-8.299	-42.641	-28.449	1.00	32.68	BBBB
ATOM	2983	CA	PRO	B	52	-12.111	-42.601	-28.453	1.00	34.43	BBBB
ATOM	2989	CA	LYS	B	53	-11.998	-39.054	-27.064	1.00	36.73	BBBB
ATOM	2998	CA	HIS	B	54	-10.116	-38.212	-30.259	1.00	34.62	BBBB
ATOM	3008	CA	GLY	B	55	-12.938	-39.481	-32.447	1.00	35.34	BBBB
ATOM	3012	CA	ILE	B	56	-10.909	-42.517	-33.514	1.00	33.81	BBBB
ATOM	3020	CA	GLU	B	57	-12.228	-46.083	-33.467	1.00	34.16	BBBB
ATOM	3029	CA	ILE	B	58	-10.217	-48.658	-31.553	1.00	31.38	BBBB
ATOM	3037	CA	ASP	B	59	-10.039	-52.442	-31.720	1.00	31.09	BBBB
ATOM	3045	CA	PHE	B	60	-8.809	-54.410	-28.713	1.00	30.32	BBBB
ATOM	3056	CA	ILE	B	61	-6.832	-57.616	-28.269	1.00	28.55	BBBB
ATOM	3064	CA	ARG	B	62	-5.709	-59.416	-25.133	1.00	30.76	BBBB
ATOM	3075	CA	ILE	B	63	-2.036	-59.770	-24.231	1.00	31.38	BBBB
ATOM	3083	CA	SER	B	64	-2.356	-60.520	-20.505	1.00	37.51	BBBB
ATOM	3089	CA	GLY	B	65	0.679	-62.355	-19.199	1.00	37.13	BBBB
ATOM	3093	CA	LEU	B	66	2.591	-61.413	-22.355	1.00	33.17	BBBB
ATOM	3101	CA	ARG	B	67	3.671	-57.928	-21.277	1.00	30.90	BBBB
ATOM	3112	CA	GLY	B	68	7.380	-57.427	-20.685	1.00	26.79	BBBB
ATOM	3116	CA	LYS	B	69	8.238	-60.463	-22.796	1.00	23.93	BBBB
ATOM	3125	CA	GLY	B	70	10.755	-60.229	-25.636	1.00	22.26	BBBB
ATOM	3129	CA	ILE	B	71	10.357	-62.386	-28.762	1.00	23.55	BBBB
ATOM	3137	CA	LYS	B	72	12.038	-65.491	-27.343	1.00	24.92	BBBB
ATOM	3146	CA	ALA	B	73	9.839	-65.306	-24.233	1.00	21.18	BBBB
ATOM	3151	CA	LEU	B	74	6.745	-64.762	-26.387	1.00	19.36	BBBB
ATOM	3159	CA	ILE	B	75	7.434	-67.768	-28.601	1.00	21.18	BBBB
ATOM	3167	CA	ALA	B	76	7.996	-69.726	-25.374	1.00	21.72	BBBB
ATOM	3172	CA	ALA	B	77	4.289	-69.121	-24.655	1.00	21.07	BBBB
ATOM	3178	CA	PRO	B	78	2.772	-70.846	-27.771	1.00	20.95	BBBB
ATOM	3184	CA	LEU	B	79	-0.896	-70.728	-26.783	1.00	21.32	BBBB
ATOM	3192	CA	ARG	B	80	-0.980	-67.115	-25.637	1.00	21.30	BBBB
ATOM	3203	CA	ILE	B	81	1.113	-65.621	-28.421	1.00	19.47	BBBB
ATOM	3211	CA	PHE	B	82	-0.875	-67.582	-31.038	1.00	19.15	BBBB
ATOM	3222	CA	ASN	B	83	-4.150	-66.332	-29.577	1.00	20.90	BBBB
ATOM	3230	CA	ALA	B	84	-3.177	-62.647	-29.484	1.00	19.30	BBBB
ATOM	3235	CA	TRP	B	85	-1.820	-63.111	-33.032	1.00	20.56	BBBB
ATOM	3249	CA	ARG	B	86	-5.140	-64.660	-34.166	1.00	23.28	BBBB
ATOM	3260	CA	GLN	B	87	-7.101	-61.802	-32.567	1.00	24.07	BBBB
ATOM	3269	CA	ALA	B	88	-4.996	-59.183	-34.355	1.00	23.78	BBBB
ATOM	3274	CA	ARG	B	89	-5.285	-61.111	-37.636	1.00	24.94	BBBB
ATOM	3285	CA	ALA	B	90	-9.088	-61.151	-37.383	1.00	26.16	BBBB
ATOM	3290	CA	ILE	B	91	-9.108	-57.400	-36.733	1.00	26.97	BBBB
ATOM	3298	CA	MET	B	92	-6.872	-56.693	-39.717	1.00	29.03	BBBB
ATOM	3306	CA	LYS	B	93	-8.735	-59.038	-42.050	1.00	33.20	BBBB
ATOM	3315	CA	ALA	B	94	-11.943	-57.157	-41.183	1.00	33.62	BBBB
ATOM	3320	CA	TYR	B	95	-10.504	-53.620	-41.224	1.00	33.83	BBBB
ATOM	3332	CA	LYS	B	96	-8.104	-54.327	-44.122	1.00	33.85	BBBB
ATOM	3342	CA	PRO	B	97	-5.490	-51.623	-43.419	1.00	31.82	BBBB
ATOM	3348	CA	ASP	B	98	-3.049	-50.685	-46.188	1.00	29.78	BBBB
ATOM	3356	CA	VAL	B	99	-0.296	-50.214	-43.660	1.00	26.75	BBBB
ATOM	3363	CA	VAL	B	100	0.227	-50.613	-39.936	1.00	23.59	BBBB
ATOM	3370	CA	LEU	B	101	2.214	-48.199	-37.797	1.00	21.59	BBBB
ATOM	3378	CA	GLY	B	102	3.796	-49.357	-34.549	1.00	19.23	BBBB
ATOM	3382	CA	MET	B	103	4.892	-46.597	-32.191	1.00	18.93	BBBB
ATOM	3389	N	GLY	B	104	5.640	-48.450	-30.827	1.00	21.56	BBBB
ATOM	3390	CA	GLY	B	104	6.275	-49.080	-29.686	1.00	21.89	BBBB
ATOM	3391	C	GLY	B	104	5.192	-49.614	-28.764	1.00	23.28	BBBB
ATOM	3392	O	GLY	B	104	4.009	-49.353	-28.980	1.00	22.50	BBBB
ATOM	3394	CA	GLY	B	105	4.593	-50.905	-26.827	1.00	23.54	BBBB
ATOM	3398	CA	TYR	B	106	3.818	-54.554	-26.159	1.00	22.37	BBBB
ATOM	3410	CA	VAL	B	107	0.557	-54.694	-28.099	1.00	18.06	BBBB
ATOM	3417	CA	SER	B	108	2.488	-53.892	-31.290	1.00	19.67	BBBB
ATOM	3423	CA	GLY	B	109	4.251	-57.256	-31.023	1.00	20.03	BBBB
ATOM	3428	CA	PRO	B	110	1.251	-59.478	-31.855	1.00	18.99	BBBB
ATOM	3434	CA	GLY	B	111	-0.160	-56.702	-34.025	1.00	19.60	BBBB
ATOM	3438	CA	GLY	B	112	3.014	-56.417	-36.074	1.00	19.97	BBBB

ATOM	3442	CA	LEU	B	113	3.265	-60.184	-36.429	1.00	19.49	BBBB
ATOM	3450	CA	ALA	B	114	-0.334	-60.292	-37.661	1.00	18.70	BBBB
ATOM	3455	CA	ALA	B	115	0.167	-57.516	-40.229	1.00	21.84	BBBB
ATOM	3460	CA	TRP	B	116	3.365	-59.126	-41.478	1.00	23.22	BBBB
ATOM	3474	CA	SER	B	117	1.735	-62.573	-41.873	1.00	22.61	BBBB
ATOM	3480	CA	LEU	B	118	-1.069	-60.957	-43.882	1.00	25.70	BBBB
ATOM	3488	CA	GLY	B	119	1.354	-59.174	-46.192	1.00	27.80	BBBB
ATOM	3492	CA	ILE	B	120	0.568	-55.744	-44.731	1.00	24.85	BBBB
ATOM	3501	CA	PRO	B	121	3.625	-53.477	-44.591	1.00	22.63	BBBB
ATOM	3507	CA	VAL	B	122	4.743	-52.594	-41.083	1.00	22.03	BBBB
ATOM	3514	CA	VAL	B	123	6.200	-49.184	-40.310	1.00	20.82	BBBB
ATOM	3521	CA	LEU	B	124	7.749	-48.485	-36.915	1.00	22.10	BBBB
ATOM	3528	N	HIS	B	125	8.182	-46.638	-35.447	1.00	21.40	BBBB
ATOM	3529	CA	HIS	B	125	8.814	-45.413	-34.981	1.00	21.42	BBBB
ATOM	3530	CB	HIS	B	125	7.858	-44.218	-35.067	1.00	21.57	BBBB
ATOM	3531	CG	HIS	B	125	8.432	-42.948	-34.511	1.00	23.73	BBBB
ATOM	3532	CD2	HIS	B	125	8.300	-42.368	-33.295	1.00	22.15	BBBB
ATOM	3533	ND1	HIS	B	125	9.274	-42.127	-35.236	1.00	26.23	BBBB
ATOM	3534	CE1	HIS	B	125	9.631	-41.095	-34.490	1.00	24.20	BBBB
ATOM	3535	NE2	HIS	B	125	9.054	-41.218	-33.307	1.00	26.07	BBBB
ATOM	3536	C	HIS	B	125	9.196	-45.642	-33.519	1.00	21.70	BBBB
ATOM	3537	O	HIS	B	125	8.378	-46.117	-32.725	1.00	19.81	BBBB
ATOM	3538	N	GLU	B	126	10.444	-45.332	-33.186	1.00	21.20	BBBB
ATOM	3539	CA	GLU	B	126	10.947	-45.452	-31.817	1.00	22.15	BBBB
ATOM	3540	CB	GLU	B	126	12.252	-46.246	-31.790	1.00	21.99	BBBB
ATOM	3541	CG	GLU	B	126	12.958	-46.206	-30.439	1.00	22.04	BBBB
ATOM	3542	CD	GLU	B	126	12.119	-46.824	-29.338	1.00	21.43	BBBB
ATOM	3543	OE1	GLU	B	126	11.767	-48.014	-29.471	1.00	21.92	BBBB
ATOM	3544	OE2	GLU	B	126	11.807	-46.124	-28.349	1.00	21.08	BBBB
ATOM	3545	C	GLU	B	126	11.205	-44.027	-31.326	1.00	21.93	BBBB
ATOM	3546	O	GLU	B	126	12.016	-43.300	-31.908	1.00	21.33	BBBB
ATOM	3548	CA	GLN	B	127	10.682	-42.270	-29.735	1.00	22.81	BBBB
ATOM	3557	CA	ASN	B	128	13.406	-43.097	-27.216	1.00	22.96	BBBB
ATOM	3565	CA	GLY	B	129	17.203	-43.019	-27.294	1.00	25.36	BBBB
ATOM	3569	CA	ILE	B	130	17.160	-46.716	-26.488	1.00	28.00	BBBB
ATOM	3577	CA	ALA	B	131	14.978	-49.139	-28.461	1.00	25.88	BBBB
ATOM	3582	CA	GLY	B	132	12.007	-50.532	-26.568	1.00	24.05	BBBB
ATOM	3586	CA	LEU	B	133	11.903	-54.293	-26.020	1.00	24.54	BBBB
ATOM	3594	CA	THR	B	134	9.202	-54.860	-28.639	1.00	21.22	BBBB
ATOM	3601	CA	ASN	B	135	10.407	-52.419	-31.324	1.00	20.50	BBBB
ATOM	3609	CA	LYS	B	136	13.886	-53.949	-31.144	1.00	22.79	BBBB
ATOM	3618	CA	TRP	B	137	12.753	-57.345	-32.424	1.00	22.06	BBBB
ATOM	3632	CA	LEU	B	138	9.744	-56.188	-34.431	1.00	23.15	BBBB
ATOM	3640	CA	ALA	B	139	12.128	-54.092	-36.542	1.00	25.29	BBBB
ATOM	3645	CA	LYS	B	140	13.279	-57.337	-38.182	1.00	28.05	BBBB
ATOM	3654	CA	ILE	B	141	9.963	-57.818	-40.016	1.00	26.09	BBBB
ATOM	3662	CA	ALA	B	142	9.331	-54.107	-40.498	1.00	25.03	BBBB
ATOM	3667	CA	THR	B	143	9.262	-52.595	-43.984	1.00	26.10	BBBB
ATOM	3674	CA	LYS	B	144	10.436	-49.238	-42.618	1.00	24.73	BBBB
ATOM	3683	CA	VAL	B	145	11.947	-48.311	-39.252	1.00	23.62	BBBB
ATOM	3690	CA	MET	B	146	12.338	-44.736	-37.993	1.00	23.15	BBBB
ATOM	3698	CA	GLN	B	147	13.762	-43.418	-34.712	1.00	25.05	BBBB
ATOM	3707	CA	ALA	B	148	13.559	-40.032	-33.009	1.00	26.88	BBBB
ATOM	3712	CA	PHE	B	149	17.239	-39.820	-32.098	1.00	29.39	BBBB
ATOM	3724	CA	PRO	B	150	20.310	-41.541	-33.535	1.00	31.87	BBBB
ATOM	3730	CA	GLY	B	151	21.629	-44.537	-31.595	1.00	32.62	BBBB
ATOM	3734	CA	ALA	B	152	18.447	-46.476	-30.753	1.00	32.71	BBBB
ATOM	3739	CA	PHE	B	153	18.925	-48.506	-33.937	1.00	34.83	BBBB
ATOM	3751	CA	PRO	B	154	22.158	-48.751	-35.993	1.00	38.97	BBBB
ATOM	3757	CA	ASN	B	155	20.765	-47.568	-39.346	1.00	41.08	BBBB
ATOM	3765	CA	ALA	B	156	17.170	-46.407	-38.843	1.00	37.55	BBBB
ATOM	3770	CA	GLU	B	157	16.367	-43.044	-40.460	1.00	34.40	BBBB
ATOM	3779	CA	VAL	B	158	16.337	-40.344	-37.764	1.00	31.16	BBBB
ATOM	3786	CA	VAL	B	159	13.155	-38.265	-37.889	1.00	28.10	BBBB
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ATOM	3797	CA	ASN	B	161	9.456	-36.807	-32.375	1.00	25.27	BBBB

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ATOM   3806  CA  PRO B 162       6.315 -34.747 -33.004  1.00 26.14  BBBB
ATOM   3812  CA  VAL B 163       6.456 -31.379 -31.216  1.00 27.75  BBBB
ATOM   3819  CA  ARG B 164       3.667 -28.953 -30.246  1.00 32.36  BBBB
ATOM   3830  CA  THR B 165       3.038 -26.307 -32.924  1.00 31.74  BBBB
ATOM   3837  CA  ASP B 166       3.252 -23.404 -30.466  1.00 30.64  BBBB
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ATOM   3852  CA  LEU B 168       7.780 -25.002 -33.075  1.00 28.46  BBBB
ATOM   3860  CA  ALA B 169       6.580 -21.455 -33.756  1.00 31.43  BBBB
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ATOM   3874  CA  PRO B 171      11.611 -17.457 -32.642  1.00 30.11  BBBB
ATOM   3880  CA  LEU B 172      15.157 -18.780 -33.062  1.00 28.33  BBBB
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ATOM   3913  CA  ARG B 176      14.611 -14.635 -28.525  1.00 29.01  BBBB
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ATOM   3932  CA  ALA B 178      18.766 -10.776 -28.131  1.00 30.78  BBBB
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ATOM   3941  CA  ARG B 180      18.676  -9.965 -22.787  1.00 28.97  BBBB
ATOM   3952  CA  GLU B 181      20.545  -9.027 -19.621  1.00 31.79  BBBB
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ATOM   3979  CA  ARG B 185      15.873 -17.216 -16.011  1.00 17.62  BBBB
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ATOM   4020  C   GLY B 190       6.808 -32.026 -13.604  1.00 29.67  BBBB
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ATOM   4024  C   GLY B 191       3.676 -32.104 -14.269  1.00 33.11  BBBB
ATOM   4025  O   GLY B 191       3.691 -31.556 -13.165  1.00 32.14  BBBB
ATOM   4026  N   SER B 192       2.587 -32.673 -14.779  1.00 34.23  BBBB
ATOM   4027  CA  SER B 192       1.313 -32.665 -14.064  1.00 35.91  BBBB
ATOM   4028  CB  SER B 192       0.283 -33.532 -14.801  1.00 36.87  BBBB
ATOM   4029  OG  SER B 192       0.702 -34.887 -14.877  1.00 39.58  BBBB
ATOM   4030  C   SER B 192       1.419 -33.128 -12.609  1.00 36.41  BBBB
ATOM   4031  O   SER B 192       0.862 -32.499 -11.714  1.00 35.78  BBBB
ATOM   4033  CA  GLN B 193       2.292 -34.763 -11.033  1.00 38.53  BBBB
ATOM   4041  N   GLY B 194       4.291 -33.398 -10.986  1.00 36.47  BBBB
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ATOM   4043  C   GLY B 194       6.584 -33.630 -10.146  1.00 34.51  BBBB
ATOM   4044  O   GLY B 194       6.442 -34.851 -10.191  1.00 34.26  BBBB
ATOM   4045  N   ALA B 195       7.761 -33.045  -9.938  1.00 33.54  BBBB
ATOM   4046  CA  ALA B 195       8.977 -33.819  -9.709  1.00 33.12  BBBB
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ATOM   4048  C   ALA B 195       9.423 -33.590  -8.267  1.00 32.87  BBBB
ATOM   4049  O   ALA B 195       9.955 -32.533  -7.923  1.00 31.47  BBBB
ATOM   4051  CA  ARG B 196       9.538 -34.512  -6.010  1.00 32.63  BBBB
ATOM   4062  CA  ILE B 197      13.329 -34.168  -6.164  1.00 28.10  BBBB
ATOM   4070  CA  LEU B 198      13.069 -30.833  -8.003  1.00 26.58  BBBB
ATOM   4078  CA  ASN B 199      10.497 -29.447  -5.563  1.00 27.07  BBBB
ATOM   4086  CA  GLN B 200      12.955 -30.326  -2.794  1.00 30.10  BBBB
ATOM   4095  CA  THR B 201      16.215 -29.345  -4.474  1.00 27.34  BBBB
ATOM   4102  CA  MET B 202      15.567 -26.048  -6.268  1.00 23.68  BBBB
ATOM   4111  CA  PRO B 203      14.608 -23.963  -3.220  1.00 23.84  BBBB
ATOM   4117  CA  GLN B 204      18.033 -24.708  -1.684  1.00 26.34  BBBB
ATOM   4126  CA  VAL B 205      19.672 -24.033  -5.043  1.00 24.44  BBBB
ATOM   4133  CA  ALA B 206      17.980 -20.610  -5.013  1.00 22.84  BBBB
ATOM   4138  CA  ALA B 207      19.442 -19.857  -1.576  1.00 26.65  BBBB
ATOM   4143  CA  LYS B 208      22.915 -20.595  -2.919  1.00 28.31  BBBB
ATOM   4152  CA  LEU B 209      22.577 -18.640  -6.171  1.00 25.68  BBBB
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ATOM	4164	CA	ASP	B	211	20.370	-12.647	-7.190	1.00	28.28	BBBB
ATOM	4172	CA	SER	B	212	22.098	-14.474	-10.067	1.00	25.73	BBBB
ATOM	4178	CA	VAL	B	213	18.925	-16.308	-11.116	1.00	20.76	BBBB
ATOM	4185	CA	THR	B	214	15.204	-15.726	-11.337	1.00	19.60	BBBB
ATOM	4192	CA	ILE	B	215	13.076	-18.850	-11.169	1.00	18.75	BBBB
ATOM	4200	CA	TRP	B	216	9.661	-19.973	-12.378	1.00	19.34	BBBB
ATOM	4214	CA	HIS	B	217	9.015	-23.303	-10.680	1.00	21.06	BBBB
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ATOM	4233	CA	SER	B	219	5.463	-27.800	-8.684	1.00	26.73	BBBB
ATOM	4239	CA	GLY	B	220	2.855	-30.242	-9.961	1.00	30.53	BBBB
ATOM	4243	CA	LYS	B	221	-0.657	-30.914	-8.628	1.00	35.12	BBBB
ATOM	4252	CA	GLY	B	222	-1.195	-29.899	-5.011	1.00	35.34	BBBB
ATOM	4256	CA	SER	B	223	2.451	-28.934	-4.418	1.00	33.98	BBBB
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ATOM	4271	CA	GLN	B	225	1.823	-24.239	-1.519	1.00	32.32	BBBB
ATOM	4280	CA	SER	B	226	4.701	-26.309	-0.122	1.00	28.30	BBBB
ATOM	4286	CA	VAL	B	227	7.214	-25.247	-2.791	1.00	24.28	BBBB
ATOM	4293	CA	GLU	B	228	6.178	-21.592	-2.387	1.00	27.23	BBBB
ATOM	4302	CA	GLN	B	229	6.853	-22.046	1.329	1.00	28.38	BBBB
ATOM	4311	CA	ALA	B	230	10.185	-23.754	0.682	1.00	26.18	BBBB
ATOM	4316	CA	TYR	B	231	11.371	-20.766	-1.366	1.00	25.47	BBBB
ATOM	4328	CA	ALA	B	232	10.342	-18.322	1.368	1.00	27.51	BBBB
ATOM	4333	CA	GLU	B	233	12.145	-20.441	3.966	1.00	30.87	BBBB
ATOM	4342	CA	ALA	B	234	15.215	-20.417	1.714	1.00	28.48	BBBB
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ATOM	4351	CA	GLN	B	236	14.121	-16.198	-1.870	1.00	25.53	BBBB
ATOM	4361	CA	PRO	B	237	10.336	-15.587	-1.720	1.00	24.65	BBBB
ATOM	4367	CA	GLN	B	238	10.277	-13.558	-4.945	1.00	24.29	BBBB
ATOM	4376	CA	HIS	B	239	10.526	-16.608	-7.201	1.00	22.08	BBBB
ATOM	4386	CA	LYS	B	240	7.375	-17.589	-9.105	1.00	23.26	BBBB
ATOM	4395	CA	VAL	B	241	5.740	-20.911	-8.277	1.00	23.78	BBBB
ATOM	4402	CA	THR	B	242	2.758	-22.301	-10.177	1.00	25.93	BBBB
ATOM	4409	CA	GLU	B	243	0.999	-25.651	-9.837	1.00	27.03	BBBB
ATOM	4418	CA	PHE	B	244	0.964	-26.068	-13.620	1.00	26.54	BBBB
ATOM	4429	CA	ILE	B	245	1.932	-24.242	-16.802	1.00	28.48	BBBB
ATOM	4437	CA	ASP	B	246	-0.754	-24.396	-19.457	1.00	36.00	BBBB
ATOM	4445	CA	ASP	B	247	1.245	-22.392	-21.999	1.00	30.74	BBBB
ATOM	4453	CA	MET	B	248	4.625	-24.136	-22.138	1.00	28.41	BBBB
ATOM	4461	CA	ALA	B	249	5.512	-22.216	-25.290	1.00	24.67	BBBB
ATOM	4466	CA	ALA	B	250	5.188	-18.933	-23.390	1.00	21.78	BBBB
ATOM	4471	CA	ALA	B	251	7.301	-20.259	-20.501	1.00	20.85	BBBB
ATOM	4476	CA	TYR	B	252	9.972	-21.616	-22.886	1.00	22.78	BBBB
ATOM	4488	CA	ALA	B	253	10.131	-18.224	-24.636	1.00	23.54	BBBB
ATOM	4493	CA	TRP	B	254	10.829	-16.534	-21.303	1.00	19.76	BBBB
ATOM	4507	CA	ALA	B	255	13.399	-19.025	-20.003	1.00	19.51	BBBB
ATOM	4512	CA	ASP	B	256	17.176	-19.026	-20.434	1.00	17.58	BBBB
ATOM	4520	CA	VAL	B	257	17.535	-22.603	-19.194	1.00	18.53	BBBB
ATOM	4527	CA	VAL	B	258	15.208	-25.456	-18.234	1.00	19.32	BBBB
ATOM	4534	CA	VAL	B	259	15.581	-27.957	-15.374	1.00	19.85	BBBB
ATOM	4541	CA	CYS	B	260	13.454	-31.055	-15.946	1.00	22.00	BBBB
ATOM	4546	N	ARG	B	261	12.937	-33.397	-16.212	1.00	22.34	BBBB
ATOM	4547	CA	ARG	B	261	13.170	-34.800	-16.515	1.00	23.75	BBBB
ATOM	4548	CB	ARG	B	261	11.964	-35.663	-16.104	1.00	27.16	BBBB
ATOM	4549	CG	ARG	B	261	11.376	-35.337	-14.738	1.00	31.82	BBBB
ATOM	4550	CD	ARG	B	261	11.490	-36.473	-13.732	1.00	36.33	BBBB
ATOM	4551	NE	ARG	B	261	12.865	-36.721	-13.323	1.00	38.48	BBBB
ATOM	4552	CZ	ARG	B	261	13.218	-37.176	-12.125	1.00	37.25	BBBB
ATOM	4553	NH1	ARG	B	261	12.295	-37.433	-11.204	1.00	38.46	BBBB
ATOM	4554	NH2	ARG	B	261	14.499	-37.370	-11.848	1.00	36.79	BBBB
ATOM	4555	C	ARG	B	261	13.351	-34.871	-18.032	1.00	23.98	BBBB
ATOM	4556	O	ARG	B	261	13.117	-33.883	-18.746	1.00	22.44	BBBB
ATOM	4558	CA	SER	B	262	13.975	-36.189	-19.948	1.00	23.18	BBBB
ATOM	4563	N	GLY	B	263	11.850	-37.151	-20.619	1.00	22.74	BBBB
ATOM	4564	CA	GLY	B	263	11.026	-38.079	-21.361	1.00	22.85	BBBB
ATOM	4565	C	GLY	B	263	11.392	-37.793	-22.813	1.00	24.06	BBBB

ATOM	4566	O	GLY	B	263	11.908	-36.705	-23.121	1.00	22.75	BBBB
ATOM	4567	N	ALA	B	264	11.130	-38.739	-23.708	1.00	23.37	BBBB
ATOM	4568	CA	ALA	B	264	11.482	-38.564	-25.115	1.00	24.25	BBBB
ATOM	4569	CB	ALA	B	264	11.133	-39.829	-25.894	1.00	24.58	BBBB
ATOM	4570	C	ALA	B	264	10.843	-37.343	-25.783	1.00	24.29	BBBB
ATOM	4571	O	ALA	B	264	11.523	-36.572	-26.470	1.00	24.33	BBBB
ATOM	4573	CA	LEU	B	265	8.846	-36.037	-26.205	1.00	24.66	BBBB
ATOM	4581	CA	THR	B	266	10.194	-33.557	-23.657	1.00	22.34	BBBB
ATOM	4588	CA	VAL	B	267	13.730	-33.762	-25.023	1.00	21.11	BBBB
ATOM	4595	CA	SER	B	268	12.411	-33.191	-28.567	1.00	21.96	BBBB
ATOM	4600	N	GLU	B	269	10.928	-31.563	-27.557	1.00	21.64	BBBB
ATOM	4601	CA	GLU	B	269	10.282	-30.272	-27.378	1.00	21.95	BBBB
ATOM	4602	CB	GLU	B	269	9.213	-30.399	-26.292	1.00	24.72	BBBB
ATOM	4603	CG	GLU	B	269	8.480	-29.128	-25.940	1.00	27.67	BBBB
ATOM	4604	CD	GLU	B	269	7.385	-29.380	-24.908	1.00	30.05	BBBB
ATOM	4605	OE1	GLU	B	269	6.325	-29.915	-25.287	1.00	31.50	BBBB
ATOM	4606	OE2	GLU	B	269	7.591	-29.057	-23.719	1.00	29.84	BBBB
ATOM	4607	C	GLU	B	269	11.321	-29.214	-26.999	1.00	21.68	BBBB
ATOM	4608	O	GLU	B	269	11.301	-28.095	-27.518	1.00	18.12	BBBB
ATOM	4610	CA	ILE	B	270	13.295	-28.698	-25.638	1.00	20.62	BBBB
ATOM	4618	CA	ALA	B	271	15.440	-29.058	-28.776	1.00	22.45	BBBB
ATOM	4623	CA	ALA	B	272	12.719	-27.451	-30.898	1.00	22.17	BBBB
ATOM	4628	CA	ALA	B	273	12.361	-24.596	-28.407	1.00	21.97	BBBB
ATOM	4633	CA	GLY	B	274	16.093	-24.023	-28.709	1.00	21.07	BBBB
ATOM	4637	CA	LEU	B	275	16.666	-24.057	-24.966	1.00	19.78	BBBB
ATOM	4646	CA	PRO	B	276	19.651	-25.199	-22.875	1.00	16.62	BBBB
ATOM	4652	CA	ALA	B	277	18.638	-27.807	-20.321	1.00	15.80	BBBB
ATOM	4657	CA	LEU	B	278	19.896	-29.429	-17.145	1.00	18.48	BBBB
ATOM	4665	CA	PHE	B	279	18.266	-32.838	-17.392	1.00	21.59	BBBB
ATOM	4676	CA	VAL	B	280	17.502	-34.902	-14.281	1.00	25.67	BBBB
ATOM	4682	N	PRO	B	281	17.324	-37.080	-15.370	1.00	27.08	BBBB
ATOM	4683	CD	PRO	B	281	18.750	-37.057	-15.726	1.00	27.31	BBBB
ATOM	4684	CA	PRO	B	281	16.698	-38.320	-15.824	1.00	29.05	BBBB
ATOM	4685	CB	PRO	B	281	17.851	-39.071	-16.492	1.00	29.44	BBBB
ATOM	4686	CG	PRO	B	281	18.791	-37.992	-16.895	1.00	29.67	BBBB
ATOM	4687	C	PRO	B	281	16.092	-39.121	-14.684	1.00	31.51	BBBB
ATOM	4688	O	PRO	B	281	16.675	-39.223	-13.603	1.00	32.26	BBBB
ATOM	4690	CA	PHE	B	282	14.246	-40.496	-13.926	1.00	37.13	BBBB
ATOM	4701	CA	GLN	B	283	16.319	-43.395	-12.591	1.00	41.11	BBBB
ATOM	4710	CA	HIS	B	284	15.641	-46.917	-13.843	1.00	43.69	BBBB
ATOM	4720	CA	LYS	B	285	17.767	-49.993	-14.571	1.00	45.34	BBBB
ATOM	4729	CA	ASP	B	286	16.949	-49.299	-18.222	1.00	43.26	BBBB
ATOM	4737	CA	ARG	B	287	17.951	-45.623	-17.883	1.00	36.28	BBBB
ATOM	4748	CA	GLN	B	288	15.622	-44.804	-20.755	1.00	30.77	BBBB
ATOM	4756	N	GLN	B	289	15.378	-42.554	-19.857	1.00	29.38	BBBB
ATOM	4757	CA	GLN	B	289	15.474	-41.099	-19.904	1.00	29.46	BBBB
ATOM	4758	CB	GLN	B	289	14.772	-40.472	-18.700	1.00	29.25	BBBB
ATOM	4759	CG	GLN	B	289	13.265	-40.416	-18.883	1.00	29.32	BBBB
ATOM	4760	CD	GLN	B	289	12.575	-39.585	-17.826	1.00	29.84	BBBB
ATOM	4761	OE1	GLN	B	289	13.191	-38.728	-17.188	1.00	29.52	BBBB
ATOM	4762	NE2	GLN	B	289	11.281	-39.821	-17.647	1.00	28.95	BBBB
ATOM	4763	C	GLN	B	289	16.906	-40.613	-20.005	1.00	29.36	BBBB
ATOM	4764	O	GLN	B	289	17.173	-39.557	-20.585	1.00	29.12	BBBB
ATOM	4766	CA	TYR	B	290	19.228	-40.984	-19.550	1.00	29.55	BBBB
ATOM	4778	CA	TRP	B	291	19.542	-42.282	-23.116	1.00	28.07	BBBB
ATOM	4791	N	ASN	B	292	17.658	-40.779	-23.508	1.00	25.52	BBBB
ATOM	4792	CA	ASN	B	292	16.902	-39.784	-24.270	1.00	26.06	BBBB
ATOM	4793	CB	ASN	B	292	15.484	-39.599	-23.709	1.00	24.78	BBBB
ATOM	4794	CG	ASN	B	292	14.590	-40.811	-23.928	1.00	24.46	BBBB
ATOM	4795	OD1	ASN	B	292	14.842	-41.641	-24.798	1.00	25.33	BBBB
ATOM	4796	ND2	ASN	B	292	13.523	-40.900	-23.146	1.00	23.83	BBBB
ATOM	4797	C	ASN	B	292	17.605	-38.427	-24.258	1.00	25.99	BBBB
ATOM	4798	O	ASN	B	292	17.566	-37.687	-25.244	1.00	26.18	BBBB
ATOM	4799	N	ALA	B	293	18.242	-38.105	-23.139	1.00	25.66	BBBB
ATOM	4800	CA	ALA	B	293	18.926	-36.822	-22.979	1.00	25.69	BBBB
ATOM	4801	CB	ALA	B	293	18.940	-36.422	-21.506	1.00	24.17	BBBB

ATOM	4802	C	ALA	B	293	20.346	-36.800	-23.521	1.00	25.67	BBBB
ATOM	4803	O	ALA	B	293	20.855	-35.743	-23.902	1.00	25.52	BBBB
ATOM	4805	CA	LEU	B	294	22.354	-38.088	-24.032	1.00	25.90	BBBB
ATOM	4814	CA	PRO	B	295	21.998	-36.870	-27.635	1.00	26.15	BBBB
ATOM	4820	CA	LEU	B	296	21.521	-33.265	-26.481	1.00	25.42	BBBB
ATOM	4828	CA	GLU	B	297	24.354	-33.530	-23.953	1.00	28.78	BBBB
ATOM	4837	CA	LYS	B	298	26.644	-34.947	-26.648	1.00	31.90	BBBB
ATOM	4846	CA	ALA	B	299	25.773	-31.965	-28.847	1.00	30.38	BBBB
ATOM	4851	CA	GLY	B	300	26.777	-29.635	-26.017	1.00	26.18	BBBB
ATOM	4855	CA	ALA	B	301	23.214	-28.333	-25.638	1.00	22.50	BBBB
ATOM	4860	CA	ALA	B	302	22.516	-29.770	-22.186	1.00	21.78	BBBB
ATOM	4865	CA	LYS	B	303	23.979	-31.340	-19.048	1.00	25.86	BBBB
ATOM	4874	CA	ILE	B	304	22.753	-34.598	-17.550	1.00	27.17	BBBB
ATOM	4882	CA	ILE	B	305	22.843	-35.178	-13.813	1.00	29.01	BBBB
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ATOM	4899	CA	GLN	B	307	20.377	-39.599	-9.613	1.00	40.54	BBBB
ATOM	4909	CA	PRO	B	308	23.828	-40.891	-8.484	1.00	43.20	BBBB
ATOM	4915	CA	GLN	B	309	25.247	-37.361	-8.787	1.00	43.46	BBBB
ATOM	4924	CA	LEU	B	310	22.232	-35.166	-8.022	1.00	39.65	BBBB
ATOM	4932	CA	SER	B	311	22.660	-32.714	-5.154	1.00	34.90	BBBB
ATOM	4938	CA	VAL	B	312	21.990	-29.074	-4.341	1.00	31.50	BBBB
ATOM	4945	CA	ASP	B	313	25.642	-28.202	-4.957	1.00	29.61	BBBB
ATOM	4953	CA	ALA	B	314	25.782	-30.099	-8.254	1.00	26.47	BBBB
ATOM	4958	CA	VAL	B	315	22.755	-28.215	-9.612	1.00	25.33	BBBB
ATOM	4965	CA	ALA	B	316	23.888	-24.872	-8.199	1.00	27.13	BBBB
ATOM	4970	CA	ASN	B	317	27.444	-25.246	-9.518	1.00	28.52	BBBB
ATOM	4978	CA	THR	B	318	26.174	-26.371	-12.906	1.00	27.04	BBBB
ATOM	4985	CA	LEU	B	319	23.883	-23.370	-13.357	1.00	25.21	BBBB
ATOM	4993	CA	ALA	B	320	26.445	-20.931	-11.957	1.00	24.59	BBBB
ATOM	4998	CA	GLY	B	321	28.934	-22.031	-14.591	1.00	24.34	BBBB
ATOM	5002	CA	TRP	B	322	26.738	-21.007	-17.521	1.00	21.72	BBBB
ATOM	5016	CA	SER	B	323	27.141	-17.404	-18.692	1.00	19.04	BBBB
ATOM	5022	CA	ARG	B	324	24.725	-15.741	-21.112	1.00	18.09	BBBB
ATOM	5033	CA	GLU	B	325	27.220	-16.368	-23.954	1.00	16.96	BBBB
ATOM	5042	CA	THR	B	326	27.460	-20.055	-23.070	1.00	16.39	BBBB
ATOM	5049	CA	LEU	B	327	23.659	-20.305	-22.780	1.00	17.27	BBBB
ATOM	5057	CA	LEU	B	328	23.175	-18.745	-26.222	1.00	17.39	BBBB
ATOM	5065	CA	THR	B	329	25.567	-21.335	-27.688	1.00	21.30	BBBB
ATOM	5072	CA	MET	B	330	23.771	-24.153	-25.870	1.00	19.91	BBBB
ATOM	5080	CA	ALA	B	331	20.412	-22.871	-27.098	1.00	18.49	BBBB
ATOM	5085	CA	GLU	B	332	21.626	-22.827	-30.704	1.00	21.47	BBBB
ATOM	5094	CA	ARG	B	333	23.040	-26.330	-30.408	1.00	23.77	BBBB
ATOM	5105	CA	ALA	B	334	19.648	-27.420	-29.063	1.00	22.88	BBBB
ATOM	5110	CA	ARG	B	335	17.795	-25.892	-32.002	1.00	23.54	BBBB
ATOM	5121	CA	ALA	B	336	20.330	-27.477	-34.372	1.00	26.85	BBBB
ATOM	5126	CA	ALA	B	337	19.740	-30.925	-32.865	1.00	30.89	BBBB
ATOM	5131	CA	SER	B	338	16.008	-30.432	-33.408	1.00	32.41	BBBB
ATOM	5137	CA	ILE	B	339	13.882	-31.941	-36.187	1.00	34.35	BBBB
ATOM	5146	CA	PRO	B	340	10.733	-29.730	-36.600	1.00	34.94	BBBB
ATOM	5152	CA	ASP	B	341	8.711	-31.820	-39.056	1.00	33.33	BBBB
ATOM	5160	CA	ALA	B	342	8.875	-35.238	-37.411	1.00	29.09	BBBB
ATOM	5165	CA	THR	B	343	5.115	-35.696	-37.744	1.00	28.55	BBBB
ATOM	5172	CA	GLU	B	344	5.085	-34.933	-41.480	1.00	32.00	BBBB
ATOM	5181	CA	ARG	B	345	8.138	-37.123	-42.067	1.00	31.44	BBBB
ATOM	5192	CA	VAL	B	346	6.578	-40.151	-40.384	1.00	28.61	BBBB
ATOM	5199	CA	ALA	B	347	3.249	-39.617	-42.137	1.00	28.96	BBBB
ATOM	5204	CA	ASN	B	348	5.035	-39.286	-45.493	1.00	34.56	BBBB
ATOM	5212	CA	GLU	B	349	6.954	-42.540	-44.956	1.00	34.86	BBBB
ATOM	5221	CA	VAL	B	350	3.767	-44.306	-43.919	1.00	33.79	BBBB
ATOM	5228	CA	SER	B	351	2.196	-42.946	-47.095	1.00	36.67	BBBB
ATOM	5234	CA	ARG	B	352	5.114	-44.088	-49.251	1.00	40.03	BBBB
ATOM	5245	CA	VAL	B	353	5.089	-47.587	-47.737	1.00	42.78	BBBB
ATOM	5252	CA	ALA	B	354	1.336	-47.957	-48.212	1.00	47.24	BBBB
ATOM	5257	CA	ARG	B	355	2.035	-46.964	-51.824	1.00	52.71	BBBB
ATOM	5268	CA	ALA	B	356	4.453	-49.913	-51.809	1.00	54.93	BBBB
ATOM	5273	CA	LEU	B	357	7.023	-47.522	-53.289	1.00	57.81	BBBB

END

TABLE 4 ATOMIC COORDINATES OF THE

DONOR NUCLEOTIDE BINDING SITE

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REMARK    4 1MUR COMPLIES WITH FORMAT V. 2.0, 11-MAY-2000
ATOM      1  N   LEU B 187      13.695 -22.128 -15.588  1.00 15.92      N
ATOM      2  CA  LEU B 187      12.361 -22.710 -15.604  1.00 16.75      C
ATOM      3  C   LEU B 187      12.450 -24.146 -15.085  1.00 16.85      C
ATOM      4  O   LEU B 187      13.115 -24.982 -15.688  1.00 17.18      O
ATOM      5  CB  LEU B 187      11.813 -22.701 -17.035  1.00 16.85      C
ATOM      6  CG  LEU B 187      10.445 -23.340 -17.276  1.00 18.63      C
ATOM      7  CD1 LEU B 187       9.368 -22.478 -16.625  1.00 19.42      C
ATOM      8  CD2 LEU B 187      10.198 -23.449 -18.783  1.00 19.11      C
ATOM      9  N   VAL B 188      11.788 -24.426 -13.964  1.00 18.20      N
ATOM     10  CA  VAL B 188      11.774 -25.775 -13.381  1.00 18.41      C
ATOM     11  C   VAL B 188      10.434 -26.440 -13.739  1.00 19.88      C
ATOM     12  O   VAL B 188       9.371 -25.967 -13.336  1.00 20.39      O
ATOM     13  CB  VAL B 188      11.902 -25.714 -11.842  1.00 18.98      C
ATOM     14  CG1 VAL B 188      12.088 -27.126 -11.270  1.00 18.50      C
ATOM     15  CG2 VAL B 188      13.061 -24.818 -11.449  1.00 18.83      C
ATOM     16  N   VAL B 189      10.493 -27.532 -14.496  1.00 21.55      N
ATOM     17  CA  VAL B 189       9.298 -28.234 -14.948  1.00 22.11      C
ATOM     18  C   VAL B 189       9.191 -29.639 -14.351  1.00 23.90      C
ATOM     19  O   VAL B 189      10.067 -30.478 -14.559  1.00 23.61      O
ATOM     20  CB  VAL B 189       9.299 -28.342 -16.488  1.00 22.50      C
ATOM     21  CG1 VAL B 189       8.009 -29.013 -16.981  1.00 22.70      C
ATOM     22  CG2 VAL B 189       9.470 -26.943 -17.101  1.00 21.26      C
ATOM     23  N   GLY B 190       8.111 -29.887 -13.615  1.00 25.60      N
ATOM     24  CA  GLY B 190       7.914 -31.188 -12.994  1.00 27.28      C
ATOM     25  C   GLY B 190       6.808 -32.026 -13.604  1.00 29.67      C
ATOM     26  O   GLY B 190       6.668 -33.208 -13.283  1.00 29.86      O
ATOM     27  N   GLY B 191       6.025 -31.430 -14.497  1.00 30.56      N
ATOM     28  CA  GLY B 191       4.935 -32.163 -15.115  1.00 31.94      C
ATOM     29  C   GLY B 191       3.676 -32.104 -14.269  1.00 33.11      C
ATOM     30  O   GLY B 191       3.691 -31.556 -13.165  1.00 32.14      O
ATOM     31  N   ALA B 195       7.761 -33.045  -9.938  1.00 33.54      N
ATOM     32  CA  ALA B 195       8.977 -33.819  -9.709  1.00 33.12      C
ATOM     33  C   ALA B 195       9.423 -33.590  -8.267  1.00 32.87      C
ATOM     34  O   ALA B 195       9.955 -32.533  -7.923  1.00 31.47      O
ATOM     35  CB  ALA B 195      10.073 -33.387 -10.679  1.00 33.17      C
ATOM     36  N   LEU B 198      12.897 -32.223  -7.590  1.00 27.07      N
ATOM     37  CA  LEU B 198      13.069 -30.833  -8.003  1.00 26.58      C
ATOM     38  C   LEU B 198      12.388 -29.893  -7.006  1.00 26.41      C
ATOM     39  O   LEU B 198      12.930 -28.835  -6.667  1.00 26.35      O
ATOM     40  CB  LEU B 198      12.504 -30.616  -9.412  1.00 25.88      C
ATOM     41  CG  LEU B 198      13.196 -31.408 -10.524  1.00 25.40      C
ATOM     42  CD1 LEU B 198      12.625 -31.007 -11.874  1.00 26.54      C
ATOM     43  CD2 LEU B 198      14.692 -31.146 -10.493  1.00 25.94      C
ATOM     44  N   TYR B 252       8.723 -21.314 -22.184  1.00 21.27      N
ATOM     45  CA  TYR B 252       9.972 -21.616 -22.886  1.00 22.78      C
ATOM     46  C   TYR B 252      10.566 -20.354 -23.516  1.00 23.57      C
ATOM     47  O   TYR B 252      11.784 -20.180 -23.550  1.00 23.91      O
ATOM     48  CB  TYR B 252       9.726 -22.661 -23.980  1.00 21.62      C
ATOM     49  CG  TYR B 252       9.662 -24.100 -23.505  1.00 23.34      C
ATOM     50  CD1 TYR B 252       9.003 -25.065 -24.261  1.00 22.88      C
ATOM     51  CD2 TYR B 252      10.288 -24.505 -22.319  1.00 22.30      C
ATOM     52  CE1 TYR B 252       8.961 -26.392 -23.861  1.00 24.81      C
ATOM     53  CE2 TYR B 252      10.253 -25.838 -21.912  1.00 23.56      C
ATOM     54  CZ  TYR B 252       9.590 -26.772 -22.687  1.00 24.26      C
ATOM     55  OH  TYR B 252       9.554 -28.088 -22.305  1.00 25.57      O
ATOM     56  N   VAL B 258      16.263 -24.643 -18.818  1.00 18.74      N
ATOM     57  CA  VAL B 258      15.208 -25.456 -18.234  1.00 19.32      C
ATOM     58  C   VAL B 258      15.799 -26.585 -17.389  1.00 19.70      C
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ATOM	59	O	VAL	B	258	16.808	-27.175	-17.758	1.00	18.96	O
ATOM	60	CB	VAL	B	258	14.328	-26.100	-19.337	1.00	19.89	C
ATOM	61	CG1	VAL	B	258	13.101	-26.757	-18.714	1.00	19.81	C
ATOM	62	CG2	VAL	B	258	13.907	-25.041	-20.364	1.00	21.59	C
ATOM	63	N	VAL	B	259	15.167	-26.861	-16.253	1.00	20.24	N
ATOM	64	CA	VAL	B	259	15.581	-27.957	-15.374	1.00	19.85	C
ATOM	65	C	VAL	B	259	14.382	-28.890	-15.371	1.00	20.02	C
ATOM	66	O	VAL	B	259	13.301	-28.500	-14.942	1.00	21.88	O
ATOM	67	CB	VAL	B	259	15.850	-27.483	-13.936	1.00	20.08	C
ATOM	68	CG1	VAL	B	259	16.222	-28.689	-13.059	1.00	20.22	C
ATOM	69	CG2	VAL	B	259	16.966	-26.453	-13.930	1.00	17.86	C
ATOM	70	N	CYS	B	260	14.562	-30.111	-15.867	1.00	21.70	N
ATOM	71	CA	CYS	B	260	13.454	-31.055	-15.946	1.00	22.00	C
ATOM	72	C	CYS	B	260	13.903	-32.478	-16.242	1.00	21.86	C
ATOM	73	O	CYS	B	260	15.087	-32.730	-16.496	1.00	21.34	O
ATOM	74	CB	CYS	B	260	12.494	-30.618	-17.057	1.00	22.77	C
ATOM	75	SG	CYS	B	260	13.297	-30.506	-18.711	1.00	22.15	S
ATOM	76	N	ARG	B	261	12.937	-33.397	-16.212	1.00	22.34	N
ATOM	77	CA	ARG	B	261	13.170	-34.800	-16.515	1.00	23.75	C
ATOM	78	C	ARG	B	261	13.351	-34.871	-18.032	1.00	23.98	C
ATOM	79	O	ARG	B	261	13.117	-33.883	-18.746	1.00	22.44	O
ATOM	80	CB	ARG	B	261	11.964	-35.663	-16.104	1.00	27.16	C
ATOM	81	CG	ARG	B	261	11.376	-35.337	-14.738	1.00	31.82	C
ATOM	82	CD	ARG	B	261	11.490	-36.473	-13.732	1.00	36.33	C
ATOM	83	NE	ARG	B	261	12.865	-36.721	-13.323	1.00	38.48	N
ATOM	84	CZ	ARG	B	261	13.218	-37.176	-12.125	1.00	37.25	C
ATOM	85	NH1	ARG	B	261	12.295	-37.433	-11.204	1.00	38.46	N
ATOM	86	NH2	ARG	B	261	14.499	-37.370	-11.848	1.00	36.79	N
ATOM	87	N	SER	B	262	13.740	-36.038	-18.527	1.00	22.00	N
ATOM	88	CA	SER	B	262	13.975	-36.189	-19.948	1.00	23.18	C
ATOM	89	C	SER	B	262	13.173	-37.263	-20.676	1.00	22.90	C
ATOM	90	O	SER	B	262	13.738	-38.179	-21.274	1.00	23.25	O
ATOM	91	CB	SER	B	262	15.481	-36.377	-20.203	1.00	24.45	C
ATOM	92	OG	SER	B	262	16.043	-37.326	-19.311	1.00	25.79	O
ATOM	93	N	GLY	B	263	11.850	-37.151	-20.619	1.00	22.74	N
ATOM	94	CA	GLY	B	263	11.026	-38.079	-21.361	1.00	22.85	C
ATOM	95	C	GLY	B	263	11.392	-37.793	-22.813	1.00	24.06	C
ATOM	96	O	GLY	B	263	11.908	-36.705	-23.121	1.00	22.75	O
ATOM	97	N	ALA	B	264	11.130	-38.739	-23.708	1.00	23.37	N
ATOM	98	CA	ALA	B	264	11.482	-38.564	-25.115	1.00	24.25	C
ATOM	99	C	ALA	B	264	10.843	-37.343	-25.783	1.00	24.29	C
ATOM	100	O	ALA	B	264	11.523	-36.572	-26.470	1.00	24.33	O
ATOM	101	CB	ALA	B	264	11.133	-39.829	-25.894	1.00	24.58	C
ATOM	102	N	LEU	B	265	9.541	-37.167	-25.596	1.00	24.44	N
ATOM	103	CA	LEU	B	265	8.846	-36.037	-26.205	1.00	24.66	C
ATOM	104	C	LEU	B	265	9.331	-34.717	-25.613	1.00	24.47	C
ATOM	105	O	LEU	B	265	9.374	-33.693	-26.301	1.00	23.85	O
ATOM	106	CB	LEU	B	265	7.332	-36.183	-26.011	1.00	25.33	C
ATOM	107	CG	LEU	B	265	6.760	-37.544	-26.426	1.00	27.97	C
ATOM	108	CD1	LEU	B	265	5.242	-37.541	-26.258	1.00	28.21	C
ATOM	109	CD2	LEU	B	265	7.146	-37.856	-27.878	1.00	27.40	C
ATOM	110	N	THR	B	266	9.702	-34.747	-24.338	1.00	22.12	N
ATOM	111	CA	THR	B	266	10.194	-33.557	-23.657	1.00	22.34	C
ATOM	112	C	THR	B	266	11.535	-33.117	-24.226	1.00	21.15	C
ATOM	113	O	THR	B	266	11.761	-31.926	-24.442	1.00	20.35	O
ATOM	114	CB	THR	B	266	10.348	-33.803	-22.140	1.00	22.35	C
ATOM	115	OG1	THR	B	266	9.061	-34.087	-21.583	1.00	24.46	O
ATOM	116	CG2	THR	B	266	10.945	-32.573	-21.444	1.00	24.00	C
ATOM	117	N	VAL	B	267	12.427	-34.075	-24.461	1.00	20.46	N
ATOM	118	CA	VAL	B	267	13.730	-33.762	-25.023	1.00	21.11	C
ATOM	119	C	VAL	B	267	13.548	-33.138	-26.416	1.00	21.34	C
ATOM	120	O	VAL	B	267	14.188	-32.135	-26.747	1.00	19.99	O
ATOM	121	CB	VAL	B	267	14.614	-35.039	-25.114	1.00	21.54	C
ATOM	122	CG1	VAL	B	267	15.903	-34.740	-25.865	1.00	20.72	C
ATOM	123	CG2	VAL	B	267	14.938	-35.541	-23.708	1.00	20.45	C
ATOM	124	N	SER	B	268	12.663	-33.717	-27.222	1.00	21.61	N

ATOM	125	CA	SER	B	268	12.411	-33.191	-28.567	1.00	21.96	C
ATOM	126	C	SER	B	268	11.817	-31.799	-28.519	1.00	21.81	C
ATOM	127	O	SER	B	268	12.158	-30.933	-29.336	1.00	22.60	O
ATOM	128	CB	SER	B	268	11.474	-34.121	-29.344	1.00	21.57	C
ATOM	129	OG	SER	B	268	12.141	-35.316	-29.721	1.00	24.06	O
ATOM	130	N	GLU	B	269	10.928	-31.563	-27.557	1.00	21.64	N
ATOM	131	CA	GLU	B	269	10.282	-30.272	-27.378	1.00	21.95	C
ATOM	132	C	GLU	B	269	11.321	-29.214	-26.999	1.00	21.68	C
ATOM	133	O	GLU	B	269	11.301	-28.095	-27.518	1.00	18.12	O
ATOM	134	CB	GLU	B	269	9.213	-30.399	-26.292	1.00	24.72	C
ATOM	135	CG	GLU	B	269	8.480	-29.128	-25.940	1.00	27.67	C
ATOM	136	CD	GLU	B	269	7.385	-29.380	-24.908	1.00	30.05	C
ATOM	137	OE1	GLU	B	269	6.325	-29.915	-25.287	1.00	31.50	O
ATOM	138	OE2	GLU	B	269	7.591	-29.057	-23.719	1.00	29.84	O
ATOM	139	N	ILE	B	270	12.224	-29.581	-26.092	1.00	19.43	N
ATOM	140	CA	ILE	B	270	13.295	-28.698	-25.638	1.00	20.62	C
ATOM	141	C	ILE	B	270	14.214	-28.314	-26.806	1.00	20.58	C
ATOM	142	O	ILE	B	270	14.595	-27.151	-26.954	1.00	20.50	O
ATOM	143	CB	ILE	B	270	14.157	-29.391	-24.533	1.00	20.30	C
ATOM	144	CG1	ILE	B	270	13.337	-29.574	-23.254	1.00	21.32	C
ATOM	145	CG2	ILE	B	270	15.415	-28.595	-24.266	1.00	19.17	C
ATOM	146	CD1	ILE	B	270	12.926	-28.291	-22.583	1.00	23.40	C
ATOM	147	N	ALA	B	277	19.316	-27.110	-21.396	1.00	17.01	N
ATOM	148	CA	ALA	B	277	18.638	-27.807	-20.321	1.00	15.80	C
ATOM	149	C	ALA	B	277	19.591	-28.526	-19.382	1.00	17.37	C
ATOM	150	O	ALA	B	277	20.710	-28.891	-19.755	1.00	17.09	O
ATOM	151	CB	ALA	B	277	17.641	-28.805	-20.895	1.00	17.01	C
ATOM	152	N	LEU	B	278	19.147	-28.673	-18.138	1.00	17.14	N
ATOM	153	CA	LEU	B	278	19.896	-29.429	-17.145	1.00	18.48	C
ATOM	154	C	LEU	B	278	18.884	-30.535	-16.898	1.00	19.62	C
ATOM	155	O	LEU	B	278	17.870	-30.330	-16.218	1.00	20.77	O
ATOM	156	CB	LEU	B	278	20.140	-28.619	-15.869	1.00	19.19	C
ATOM	157	CG	LEU	B	278	21.084	-29.308	-14.868	1.00	20.85	C
ATOM	158	CD1	LEU	B	278	21.283	-28.411	-13.668	1.00	21.11	C
ATOM	159	CD2	LEU	B	278	20.497	-30.647	-14.433	1.00	19.16	C
ATOM	160	N	PHE	B	279	19.149	-31.691	-17.495	1.00	19.50	N
ATOM	161	CA	PHE	B	279	18.266	-32.838	-17.392	1.00	21.59	C
ATOM	162	C	PHE	B	279	18.525	-33.709	-16.167	1.00	22.86	C
ATOM	163	O	PHE	B	279	19.671	-34.065	-15.871	1.00	23.32	O
ATOM	164	CB	PHE	B	279	18.385	-33.700	-18.651	1.00	21.07	C
ATOM	165	CG	PHE	B	279	17.740	-33.099	-19.876	1.00	19.35	C
ATOM	166	CD1	PHE	B	279	18.481	-32.898	-21.035	1.00	19.42	C
ATOM	167	CD2	PHE	B	279	16.379	-32.794	-19.888	1.00	18.16	C
ATOM	168	CE1	PHE	B	279	17.874	-32.405	-22.203	1.00	19.06	C
ATOM	169	CE2	PHE	B	279	15.759	-32.298	-21.052	1.00	17.65	C
ATOM	170	CZ	PHE	B	279	16.515	-32.108	-22.208	1.00	15.61	C
ATOM	171	N	VAL	B	280	17.445	-34.037	-15.461	1.00	23.88	N
ATOM	172	CA	VAL	B	280	17.502	-34.902	-14.281	1.00	25.67	C
ATOM	173	C	VAL	B	280	16.690	-36.136	-14.658	1.00	25.65	C
ATOM	174	O	VAL	B	280	15.509	-36.239	-14.346	1.00	24.57	O
ATOM	175	CB	VAL	B	280	16.883	-34.223	-13.048	1.00	26.89	C
ATOM	176	CG1	VAL	B	280	16.954	-35.159	-11.847	1.00	28.12	C
ATOM	177	CG2	VAL	B	280	17.631	-32.929	-12.742	1.00	27.70	C
ATOM	178	N	PRO	B	281	17.324	-37.080	-15.370	1.00	27.08	N
ATOM	179	CA	PRO	B	281	16.698	-38.320	-15.824	1.00	29.05	C
ATOM	180	C	PRO	B	281	16.092	-39.121	-14.684	1.00	31.51	C
ATOM	181	O	PRO	B	281	16.675	-39.223	-13.603	1.00	32.26	O
ATOM	182	CB	PRO	B	281	17.851	-39.071	-16.492	1.00	29.44	C
ATOM	183	CG	PRO	B	281	18.791	-37.992	-16.895	1.00	29.67	C
ATOM	184	CD	PRO	B	281	18.750	-37.057	-15.726	1.00	27.31	C
ATOM	185	N	PHE	B	282	14.908	-39.668	-14.923	1.00	33.83	N
ATOM	186	CA	PHE	B	282	14.246	-40.496	-13.926	1.00	37.13	C
ATOM	187	C	PHE	B	282	15.078	-41.776	-13.880	1.00	38.09	C
ATOM	188	O	PHE	B	282	15.357	-42.373	-14.921	1.00	38.33	O
ATOM	189	CB	PHE	B	282	12.818	-40.808	-14.372	1.00	38.38	C
ATOM	190	CG	PHE	B	282	12.032	-41.606	-13.377	1.00	40.57	C

ATOM	191	CD1	PHE	B	282	11.720	-41.074	-12.130	1.00	41.80	C
ATOM	192	CD2	PHE	B	282	11.590	-42.886	-13.689	1.00	41.65	C
ATOM	193	CE1	PHE	B	282	10.975	-41.806	-11.209	1.00	42.03	C
ATOM	194	CE2	PHE	B	282	10.843	-43.628	-12.773	1.00	42.49	C
ATOM	195	CZ	PHE	B	282	10.536	-43.085	-11.532	1.00	41.74	C
ATOM	196	N	GLN	B	288	16.212	-45.321	-19.533	1.00	30.94	N
ATOM	197	CA	GLN	B	288	15.622	-44.804	-20.755	1.00	30.77	C
ATOM	198	C	GLN	B	288	15.783	-43.291	-20.885	1.00	29.70	C
ATOM	199	O	GLN	B	288	16.268	-42.801	-21.902	1.00	29.79	O
ATOM	200	CB	GLN	B	288	14.143	-45.158	-20.810	1.00	30.59	C
ATOM	201	CG	GLN	B	288	13.473	-44.772	-22.109	1.00	29.73	C
ATOM	202	CD	GLN	B	288	11.981	-44.971	-22.044	1.00	28.04	C
ATOM	203	OE1	GLN	B	288	11.294	-44.295	-21.279	1.00	29.59	O
ATOM	204	NE2	GLN	B	288	11.468	-45.905	-22.838	1.00	26.98	N
ATOM	205	N	GLN	B	289	15.378	-42.554	-19.857	1.00	29.38	N
ATOM	206	CA	GLN	B	289	15.474	-41.099	-19.904	1.00	29.46	C
ATOM	207	C	GLN	B	289	16.906	-40.613	-20.005	1.00	29.36	C
ATOM	208	O	GLN	B	289	17.173	-39.557	-20.585	1.00	29.12	O
ATOM	209	CB	GLN	B	289	14.772	-40.472	-18.700	1.00	29.25	C
ATOM	210	CG	GLN	B	289	13.265	-40.416	-18.883	1.00	29.32	C
ATOM	211	CD	GLN	B	289	12.575	-39.585	-17.826	1.00	29.84	C
ATOM	212	OE1	GLN	B	289	13.191	-38.728	-17.188	1.00	29.52	O
ATOM	213	NE2	GLN	B	289	11.281	-39.821	-17.647	1.00	28.95	N
ATOM	214	N	TYR	B	290	17.835	-41.374	-19.442	1.00	28.95	N
ATOM	215	CA	TYR	B	290	19.228	-40.984	-19.550	1.00	29.55	C
ATOM	216	C	TYR	B	290	19.593	-41.042	-21.032	1.00	28.80	C
ATOM	217	O	TYR	B	290	20.192	-40.113	-21.567	1.00	29.22	O
ATOM	218	CB	TYR	B	290	20.136	-41.934	-18.768	1.00	31.40	C
ATOM	219	CG	TYR	B	290	21.587	-41.780	-19.148	1.00	33.37	C
ATOM	220	CD1	TYR	B	290	22.332	-40.682	-18.717	1.00	34.57	C
ATOM	221	CD2	TYR	B	290	22.192	-42.684	-20.017	1.00	34.90	C
ATOM	222	CE1	TYR	B	290	23.644	-40.490	-19.148	1.00	35.97	C
ATOM	223	CE2	TYR	B	290	23.497	-42.500	-20.453	1.00	36.03	C
ATOM	224	CZ	TYR	B	290	24.214	-41.402	-20.019	1.00	36.29	C
ATOM	225	OH	TYR	B	290	25.499	-41.215	-20.475	1.00	39.44	O
ATOM	226	N	ASN	B	292	17.658	-40.779	-23.508	1.00	25.52	N
ATOM	227	CA	ASN	B	292	16.902	-39.784	-24.270	1.00	26.06	C
ATOM	228	C	ASN	B	292	17.605	-38.427	-24.258	1.00	25.99	C
ATOM	229	O	ASN	B	292	17.566	-37.687	-25.244	1.00	26.18	O
ATOM	230	CB	ASN	B	292	15.484	-39.599	-23.709	1.00	24.78	C
ATOM	231	CG	ASN	B	292	14.590	-40.811	-23.928	1.00	24.46	C
ATOM	232	OD1	ASN	B	292	14.842	-41.641	-24.798	1.00	25.33	O
ATOM	233	ND2	ASN	B	292	13.523	-40.900	-23.146	1.00	23.83	N
ATOM	234	N	ALA	B	293	18.242	-38.105	-23.139	1.00	25.66	N
ATOM	235	CA	ALA	B	293	18.926	-36.822	-22.979	1.00	25.69	C
ATOM	236	C	ALA	B	293	20.346	-36.800	-23.521	1.00	25.67	C
ATOM	237	O	ALA	B	293	20.855	-35.743	-23.902	1.00	25.52	O
ATOM	238	CB	ALA	B	293	18.940	-36.422	-21.506	1.00	24.17	C
ATOM	239	N	LEU	B	296	21.375	-34.703	-26.688	1.00	25.66	N
ATOM	240	CA	LEU	B	296	21.521	-33.265	-26.481	1.00	25.42	C
ATOM	241	C	LEU	B	296	22.784	-32.935	-25.688	1.00	26.07	C
ATOM	242	O	LEU	B	296	23.435	-31.917	-25.944	1.00	25.26	O
ATOM	243	CB	LEU	B	296	20.283	-32.685	-25.779	1.00	24.45	C
ATOM	244	CG	LEU	B	296	19.066	-32.458	-26.679	1.00	25.59	C
ATOM	245	CD1	LEU	B	296	17.968	-31.718	-25.911	1.00	23.56	C
ATOM	246	CD2	LEU	B	296	19.496	-31.630	-27.893	1.00	25.87	C
ATOM	247	N	ALA	B	302	23.066	-29.504	-23.507	1.00	20.94	N
ATOM	248	CA	ALA	B	302	22.516	-29.770	-22.186	1.00	21.78	C
ATOM	249	C	ALA	B	302	23.503	-30.507	-21.288	1.00	22.69	C
ATOM	250	O	ALA	B	302	24.561	-30.948	-21.739	1.00	22.25	O
ATOM	251	CB	ALA	B	302	21.243	-30.595	-22.327	1.00	20.10	C
ATOM	252	N	LYS	B	303	23.156	-30.613	-20.009	1.00	24.62	N
ATOM	253	CA	LYS	B	303	23.979	-31.340	-19.048	1.00	25.86	C
ATOM	254	C	LYS	B	303	23.083	-32.319	-18.302	1.00	26.41	C
ATOM	255	O	LYS	B	303	22.015	-31.948	-17.802	1.00	25.76	O
ATOM	256	CB	LYS	B	303	24.632	-30.401	-18.036	1.00	27.85	C

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ATOM    257  CG  LYS B 303      25.466 -31.146 -16.986  1.00 29.37      C
ATOM    258  CD  LYS B 303      26.150 -30.186 -16.025  1.00 32.41      C
ATOM    259  CE  LYS B 303      27.083 -30.912 -15.056  1.00 33.22      C
ATOM    260  NZ  LYS B 303      27.827 -29.952 -14.181  1.00 33.62      N
ATOM    261  N   ILE B 304      23.520 -33.570 -18.234  1.00 25.65      N
ATOM    262  CA  ILE B 304      22.753 -34.598 -17.550  1.00 27.17      C
ATOM    263  C   ILE B 304      23.308 -34.855 -16.160  1.00 27.00      C
ATOM    264  O   ILE B 304      24.511 -35.012 -15.986  1.00 27.46      O
ATOM    265  CB  ILE B 304      22.786 -35.946 -18.316  1.00 27.06      C
ATOM    266  CG1 ILE B 304      22.242 -35.769 -19.733  1.00 27.61      C
ATOM    267  CG2 ILE B 304      21.977 -36.996 -17.555  1.00 28.49      C
ATOM    268  CD1 ILE B 304      22.380 -37.009 -20.599  1.00 27.05      C
ATOM    269  N   ILE B 305      22.428 -34.869 -15.168  1.00 27.22      N
ATOM    270  CA  ILE B 305      22.843 -35.178 -13.813  1.00 29.01      C
ATOM    271  C   ILE B 305      21.934 -36.302 -13.351  1.00 29.64      C
ATOM    272  O   ILE B 305      20.806 -36.067 -12.932  1.00 29.25      O
ATOM    273  CB  ILE B 305      22.713 -33.977 -12.858  1.00 28.91      C
ATOM    274  CG1 ILE B 305      23.660 -32.855 -13.299  1.00 29.51      C
ATOM    275  CG2 ILE B 305      23.063 -34.416 -11.432  1.00 30.98      C
ATOM    276  CD1 ILE B 305      23.674 -31.653 -12.367  1.00 29.43      C
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TABLE 5 ATOMIC COORDINATES OF ACCEPTOR BINDING SITE

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REMARK    4 1MUR COMPLIES WITH FORMAT V. 2.0, 11-MAY-2000
ATOM      1  N   MET B  12      -0.734 -48.902 -33.817  1.00 23.68      N
ATOM      2  CA  MET B  12      -0.523 -49.707 -32.613  1.00 24.54      C
ATOM      3  C   MET B  12       0.361 -48.840 -31.720  1.00 25.31      C
ATOM      4  O   MET B  12       1.546 -48.645 -32.006  1.00 23.88      O
ATOM      5  CB  MET B  12       0.192 -51.019 -32.971  1.00 24.28      C
ATOM      6  CG  MET B  12      -0.402 -51.726 -34.188  1.00 25.19      C
ATOM      7  SD  MET B  12       0.399 -53.284 -34.669  1.00 26.54      S
ATOM      8  CE  MET B  12       1.990 -52.691 -35.289  1.00 22.99      C
ATOM      9  N   ALA B  13      -0.224 -48.292 -30.657  1.00 27.08      N
ATOM     10  CA  ALA B  13       0.508 -47.410 -29.752  1.00 29.43      C
ATOM     11  C   ALA B  13      -0.239 -47.192 -28.436  1.00 31.80      C
ATOM     12  O   ALA B  13      -1.143 -46.350 -28.352  1.00 32.16      O
ATOM     13  CB  ALA B  13       0.747 -46.074 -30.429  1.00 28.82      C
ATOM     14  N   GLY B  14       0.150 -47.934 -27.405  1.00 32.46      N
ATOM     15  CA  GLY B  14      -0.513 -47.804 -26.120  1.00 33.82      C
ATOM     16  C   GLY B  14      -0.107 -46.595 -25.299  1.00 34.82      C
ATOM     17  O   GLY B  14       0.975 -46.040 -25.479  1.00 35.47      O
ATOM     18  N   GLY B  15      -0.986 -46.188 -24.385  1.00 35.56      N
ATOM     19  CA  GLY B  15      -0.700 -45.047 -23.536  1.00 36.08      C
ATOM     20  C   GLY B  15       0.539 -45.254 -22.683  1.00 36.84      C
ATOM     21  O   GLY B  15       1.293 -44.311 -22.426  1.00 36.03      O
ATOM     22  N   THR B  16       0.755 -46.488 -22.240  1.00 36.65      N
ATOM     23  CA  THR B  16       1.920 -46.787 -21.421  1.00 38.51      C
ATOM     24  C   THR B  16       3.158 -46.497 -22.264  1.00 38.35      C
ATOM     25  O   THR B  16       3.191 -46.798 -23.460  1.00 39.90      O
ATOM     26  CB  THR B  16       1.926 -48.258 -20.974  1.00 38.51      C
ATOM     27  OG1 THR B  16       0.686 -48.558 -20.321  1.00 38.39      O
ATOM     28  CG2 THR B  16       3.075 -48.518 -20.005  1.00 39.11      C
ATOM     29  N   GLY B  17       4.168 -45.897 -21.649  1.00 37.68      N
ATOM     30  CA  GLY B  17       5.367 -45.567 -22.392  1.00 36.57      C
ATOM     31  C   GLY B  17       5.161 -44.303 -23.211  1.00 35.56      C
ATOM     32  O   GLY B  17       6.079 -43.843 -23.890  1.00 35.03      O
ATOM     33  N   GLY B  18       3.949 -43.752 -23.150  1.00 33.83      N
ATOM     34  CA  GLY B  18       3.631 -42.529 -23.872  1.00 33.48      C
ATOM     35  C   GLY B  18       3.825 -42.593 -25.378  1.00 33.12      C
ATOM     36  O   GLY B  18       4.345 -41.650 -25.984  1.00 35.38      O
ATOM     37  N   HIS B  19       3.416 -43.699 -25.988  1.00 30.26      N
ATOM     38  CA  HIS B  19       3.548 -43.865 -27.435  1.00 28.22      C
ATOM     39  C   HIS B  19       2.280 -43.370 -28.144  1.00 27.91      C
ATOM     40  O   HIS B  19       2.300 -43.049 -29.337  1.00 26.91      O
ATOM     41  CB  HIS B  19       3.772 -45.349 -27.779  1.00 25.81      C
ATOM     42  CG  HIS B  19       4.957 -45.966 -27.094  1.00 25.35      C
ATOM     43  ND1 HIS B  19       4.845 -47.025 -26.217  1.00 24.57      N
ATOM     44  CD2 HIS B  19       6.281 -45.694 -27.184  1.00 24.18      C
ATOM     45  CE1 HIS B  19       6.046 -47.380 -25.798  1.00 23.08      C
ATOM     46  NE2 HIS B  19       6.936 -46.589 -26.369  1.00 25.51      N
ATOM     47  N   VAL B  20       1.180 -43.310 -27.402  1.00 27.65      N
ATOM     48  CA  VAL B  20      -0.098 -42.894 -27.965  1.00 27.77      C
ATOM     49  C   VAL B  20      -0.140 -41.452 -28.470  1.00 27.57      C
ATOM     50  O   VAL B  20      -0.771 -41.172 -29.486  1.00 27.12      O
ATOM     51  CB  VAL B  20      -1.248 -43.080 -26.942  1.00 28.57      C
ATOM     52  CG1 VAL B  20      -1.082 -42.114 -25.787  1.00 30.03      C
ATOM     53  CG2 VAL B  20      -2.602 -42.873 -27.631  1.00 26.82      C
ATOM     54  N   LEU B  40      -5.323 -50.004 -32.549  1.00 25.21      N
ATOM     55  CA  LEU B  40      -5.200 -51.364 -32.026  1.00 24.71      C
ATOM     56  C   LEU B  40      -4.535 -51.235 -30.655  1.00 23.33      C
ATOM     57  O   LEU B  40      -3.387 -50.824 -30.563  1.00 23.43      O
ATOM     58  CB  LEU B  40      -4.326 -52.221 -32.952  1.00 25.21      C
ATOM     59  CG  LEU B  40      -4.416 -53.754 -32.868  1.00 26.95      C
ATOM     60  CD1 LEU B  40      -3.037 -54.334 -32.571  1.00 27.63      C
ATOM     61  CD2 LEU B  40      -5.421 -54.179 -31.817  1.00 26.69      C
ATOM     62  N   GLU B  47      -4.976 -45.941 -23.678  1.00 32.85      N
ATOM     63  CA  GLU B  47      -5.458 -45.655 -25.029  1.00 31.79      C
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ATOM	64	C	GLU	B	47	-6.938	-46.017	-25.191	1.00	31.81	C
ATOM	65	O	GLU	B	47	-7.626	-45.476	-26.055	1.00	31.31	O
ATOM	66	CB	GLU	B	47	-4.624	-46.402	-26.080	1.00	30.62	C
ATOM	67	CG	GLU	B	47	-4.755	-47.922	-26.051	1.00	29.85	C
ATOM	68	CD	GLU	B	47	-3.793	-48.597	-25.082	1.00	29.78	C
ATOM	69	OE1	GLU	B	47	-3.188	-47.895	-24.247	1.00	28.76	O
ATOM	70	OE2	GLU	B	47	-3.649	-49.840	-25.156	1.00	29.01	O
ATOM	71	N	ILE	B	63	-3.428	-59.342	-24.313	1.00	30.07	N
ATOM	72	CA	ILE	B	63	-2.036	-59.770	-24.231	1.00	31.38	C
ATOM	73	C	ILE	B	63	-1.623	-59.981	-22.775	1.00	33.08	C
ATOM	74	O	ILE	B	63	-0.444	-59.872	-22.430	1.00	33.21	O
ATOM	75	CB	ILE	B	63	-1.081	-58.745	-24.883	1.00	30.06	C
ATOM	76	CG1	ILE	B	63	-1.143	-57.411	-24.137	1.00	29.94	C
ATOM	77	CG2	ILE	B	63	-1.442	-58.567	-26.353	1.00	30.41	C
ATOM	78	CD1	ILE	B	63	-0.128	-56.384	-24.632	1.00	29.62	C
ATOM	79	N	ARG	B	67	2.953	-59.185	-21.440	1.00	31.54	N
ATOM	80	CA	ARG	B	67	3.671	-57.928	-21.277	1.00	30.90	C
ATOM	81	C	ARG	B	67	5.071	-58.142	-20.713	1.00	29.99	C
ATOM	82	O	ARG	B	67	5.294	-59.034	-19.889	1.00	28.67	O
ATOM	83	CB	ARG	B	67	2.888	-56.984	-20.363	1.00	32.28	C
ATOM	84	CG	ARG	B	67	1.540	-56.576	-20.913	1.00	34.65	C
ATOM	85	CD	ARG	B	67	0.926	-55.440	-20.097	1.00	36.69	C
ATOM	86	NE	ARG	B	67	-0.259	-54.889	-20.748	1.00	38.28	N
ATOM	87	CZ	ARG	B	67	-1.425	-55.519	-20.853	1.00	39.05	C
ATOM	88	NH1	ARG	B	67	-1.583	-56.734	-20.341	1.00	39.61	N
ATOM	89	NH2	ARG	B	67	-2.434	-54.935	-21.487	1.00	39.52	N
ATOM	90	N	GLY	B	68	6.014	-57.321	-21.165	1.00	27.75	N
ATOM	91	CA	GLY	B	68	7.380	-57.427	-20.685	1.00	26.79	C
ATOM	92	C	GLY	B	68	8.166	-58.579	-21.280	1.00	25.41	C
ATOM	93	O	GLY	B	68	9.326	-58.779	-20.943	1.00	26.04	O
ATOM	94	N	GLY	B	102	3.556	-48.986	-35.936	1.00	20.96	N
ATOM	95	CA	GLY	B	102	3.796	-49.357	-34.549	1.00	19.23	C
ATOM	96	C	GLY	B	102	4.655	-48.282	-33.918	1.00	18.45	C
ATOM	97	O	GLY	B	102	5.765	-48.016	-34.381	1.00	18.70	O
ATOM	98	N	MET	B	103	4.155	-47.660	-32.857	1.00	18.01	N
ATOM	99	CA	MET	B	103	4.892	-46.597	-32.191	1.00	18.93	C
ATOM	100	C	MET	B	103	5.612	-47.128	-30.957	1.00	18.98	C
ATOM	101	O	MET	B	103	6.134	-46.357	-30.158	1.00	17.96	O
ATOM	102	CB	MET	B	103	3.928	-45.477	-31.781	1.00	20.02	C
ATOM	103	CG	MET	B	103	3.121	-44.888	-32.944	1.00	21.61	C
ATOM	104	SD	MET	B	103	4.212	-44.135	-34.157	1.00	23.45	S
ATOM	105	CE	MET	B	103	4.718	-42.680	-33.271	1.00	21.40	C
ATOM	106	N	GLY	B	104	5.640	-48.450	-30.827	1.00	21.56	N
ATOM	107	CA	GLY	B	104	6.275	-49.080	-29.686	1.00	21.89	C
ATOM	108	C	GLY	B	104	5.192	-49.614	-28.764	1.00	23.28	C
ATOM	109	O	GLY	B	104	4.009	-49.353	-28.980	1.00	22.50	O
ATOM	110	N	GLY	B	105	5.583	-50.364	-27.741	1.00	23.01	N
ATOM	111	CA	GLY	B	105	4.593	-50.905	-26.827	1.00	23.54	C
ATOM	112	C	GLY	B	105	4.358	-52.380	-27.078	1.00	23.17	C
ATOM	113	O	GLY	B	105	4.449	-52.844	-28.214	1.00	22.69	O
ATOM	114	N	TYR	B	106	4.018	-53.118	-26.026	1.00	22.87	N
ATOM	115	CA	TYR	B	106	3.818	-54.554	-26.159	1.00	22.37	C
ATOM	116	C	TYR	B	106	2.719	-55.018	-27.100	1.00	20.52	C
ATOM	117	O	TYR	B	106	2.867	-56.052	-27.746	1.00	20.50	O
ATOM	118	CB	TYR	B	106	3.632	-55.181	-24.774	1.00	25.08	C
ATOM	119	CG	TYR	B	106	4.864	-55.008	-23.929	1.00	28.19	C
ATOM	120	CD1	TYR	B	106	4.869	-54.153	-22.830	1.00	31.96	C
ATOM	121	CD2	TYR	B	106	6.058	-55.631	-24.282	1.00	31.27	C
ATOM	122	CE1	TYR	B	106	6.043	-53.915	-22.108	1.00	33.13	C
ATOM	123	CE2	TYR	B	106	7.234	-55.400	-23.569	1.00	32.27	C
ATOM	124	CZ	TYR	B	106	7.219	-54.541	-22.487	1.00	33.19	C
ATOM	125	OH	TYR	B	106	8.388	-54.291	-21.802	1.00	35.95	O
ATOM	126	N	VAL	B	107	1.628	-54.270	-27.205	1.00	19.06	N
ATOM	127	CA	VAL	B	107	0.557	-54.694	-28.099	1.00	18.06	C
ATOM	128	C	VAL	B	107	1.015	-54.743	-29.559	1.00	17.45	C
ATOM	129	O	VAL	B	107	0.502	-55.536	-30.346	1.00	16.99	O

ATOM	130	CB	VAL	B	107	-0.690	-53.774	-27.978	1.00	20.95	C
ATOM	131	CG1	VAL	B	107	-0.407	-52.407	-28.589	1.00	21.39	C
ATOM	132	CG2	VAL	B	107	-1.879	-54.433	-28.658	1.00	21.30	C
ATOM	133	N	SER	B	108	1.991	-53.916	-29.918	1.00	17.96	N
ATOM	134	CA	SER	B	108	2.488	-53.892	-31.290	1.00	19.67	C
ATOM	135	C	SER	B	108	3.197	-55.187	-31.694	1.00	20.38	C
ATOM	136	O	SER	B	108	3.385	-55.449	-32.884	1.00	21.25	O
ATOM	137	CB	SER	B	108	3.424	-52.691	-31.508	1.00	19.56	C
ATOM	138	OG	SER	B	108	4.666	-52.824	-30.837	1.00	19.63	O
ATOM	139	N	GLY	B	109	3.595	-55.995	-30.710	1.00	19.59	N
ATOM	140	CA	GLY	B	109	4.251	-57.256	-31.023	1.00	20.03	C
ATOM	141	C	GLY	B	109	3.311	-58.170	-31.792	1.00	19.61	C
ATOM	142	O	GLY	B	109	3.579	-58.517	-32.940	1.00	19.24	O
ATOM	143	N	PRO	B	110	2.206	-58.606	-31.173	1.00	19.20	N
ATOM	144	CA	PRO	B	110	1.251	-59.478	-31.855	1.00	18.99	C
ATOM	145	C	PRO	B	110	0.651	-58.761	-33.075	1.00	19.22	C
ATOM	146	O	PRO	B	110	0.406	-59.371	-34.116	1.00	17.13	O
ATOM	147	CB	PRO	B	110	0.198	-59.737	-30.778	1.00	20.41	C
ATOM	148	CG	PRO	B	110	0.998	-59.720	-29.515	1.00	19.81	C
ATOM	149	CD	PRO	B	110	1.914	-58.528	-29.729	1.00	19.94	C
ATOM	150	N	HIS	B	125	8.182	-46.638	-35.447	1.00	21.40	N
ATOM	151	CA	HIS	B	125	8.814	-45.413	-34.981	1.00	21.42	C
ATOM	152	C	HIS	B	125	9.196	-45.642	-33.519	1.00	21.70	C
ATOM	153	O	HIS	B	125	8.378	-46.117	-32.725	1.00	19.81	O
ATOM	154	CB	HIS	B	125	7.858	-44.218	-35.067	1.00	21.57	C
ATOM	155	CG	HIS	B	125	8.432	-42.948	-34.511	1.00	23.73	C
ATOM	156	ND1	HIS	B	125	9.274	-42.127	-35.236	1.00	26.23	N
ATOM	157	CD2	HIS	B	125	8.300	-42.368	-33.295	1.00	22.15	C
ATOM	158	CE1	HIS	B	125	9.631	-41.095	-34.490	1.00	24.20	C
ATOM	159	NE2	HIS	B	125	9.054	-41.218	-33.307	1.00	26.07	N
ATOM	160	N	GLU	B	126	10.444	-45.332	-33.186	1.00	21.20	N
ATOM	161	CA	GLU	B	126	10.947	-45.452	-31.817	1.00	22.15	C
ATOM	162	C	GLU	B	126	11.205	-44.027	-31.326	1.00	21.93	C
ATOM	163	O	GLU	B	126	12.016	-43.300	-31.908	1.00	21.33	O
ATOM	164	CB	GLU	B	126	12.252	-46.246	-31.790	1.00	21.99	C
ATOM	165	CG	GLU	B	126	12.958	-46.206	-30.439	1.00	22.04	C
ATOM	166	CD	GLU	B	126	12.119	-46.824	-29.338	1.00	21.43	C
ATOM	167	OE1	GLU	B	126	11.767	-48.014	-29.471	1.00	21.92	O
ATOM	168	OE2	GLU	B	126	11.807	-46.124	-28.349	1.00	21.08	O
ATOM	169	N	GLN	B	127	10.520	-43.624	-30.259	1.00	22.62	N
ATOM	170	CA	GLN	B	127	10.682	-42.270	-29.735	1.00	22.81	C
ATOM	171	C	GLN	B	127	11.874	-42.087	-28.809	1.00	22.39	C
ATOM	172	O	GLN	B	127	12.399	-40.976	-28.682	1.00	22.43	O
ATOM	173	CB	GLN	B	127	9.414	-41.814	-28.989	1.00	23.56	C
ATOM	174	CG	GLN	B	127	8.147	-41.783	-29.830	1.00	24.46	C
ATOM	175	CD	GLN	B	127	7.312	-43.041	-29.687	1.00	25.85	C
ATOM	176	OE1	GLN	B	127	6.842	-43.366	-28.591	1.00	23.78	O
ATOM	177	NE2	GLN	B	127	7.119	-43.758	-30.797	1.00	24.91	N
ATOM	178	N	ASN	B	128	12.314	-43.173	-28.177	1.00	22.35	N
ATOM	179	CA	ASN	B	128	13.406	-43.097	-27.216	1.00	22.96	C
ATOM	180	C	ASN	B	128	14.824	-43.314	-27.742	1.00	23.87	C
ATOM	181	O	ASN	B	128	15.026	-43.856	-28.830	1.00	24.05	O
ATOM	182	CB	ASN	B	128	13.136	-44.080	-26.064	1.00	22.85	C
ATOM	183	CG	ASN	B	128	11.742	-43.919	-25.474	1.00	23.25	C
ATOM	184	OD1	ASN	B	128	10.804	-44.632	-25.848	1.00	26.04	O
ATOM	185	ND2	ASN	B	128	11.597	-42.975	-24.556	1.00	22.68	N
ATOM	186	N	GLY	B	132	12.851	-49.814	-27.506	1.00	24.52	N
ATOM	187	CA	GLY	B	132	12.007	-50.532	-26.568	1.00	24.05	C
ATOM	188	C	GLY	B	132	12.150	-52.019	-26.831	1.00	23.35	C
ATOM	189	O	GLY	B	132	12.582	-52.419	-27.904	1.00	22.89	O
ATOM	190	N	LEU	B	133	11.788	-52.846	-25.860	1.00	23.38	N
ATOM	191	CA	LEU	B	133	11.903	-54.293	-26.020	1.00	24.54	C
ATOM	192	C	LEU	B	133	11.209	-54.833	-27.276	1.00	22.84	C
ATOM	193	O	LEU	B	133	11.784	-55.619	-28.027	1.00	21.86	O
ATOM	194	CB	LEU	B	133	11.328	-54.996	-24.786	1.00	25.48	C
ATOM	195	CG	LEU	B	133	11.388	-56.527	-24.780	1.00	27.50	C

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ATOM    196  CD1 LEU B 133      12.840 -56.984 -24.866  1.00 28.69      C
ATOM    197  CD2 LEU B 133      10.735 -57.053 -23.509  1.00 28.04      C
ATOM    198  N   THR B 134       9.975 -54.401 -27.499  1.00 21.72      N
ATOM    199  CA  THR B 134       9.202 -54.860 -28.639  1.00 21.22      C
ATOM    200  C   THR B 134       9.693 -54.326 -29.986  1.00 20.62      C
ATOM    201  O   THR B 134       9.843 -55.091 -30.932  1.00 20.33      O
ATOM    202  CB  THR B 134       7.716 -54.509 -28.449  1.00 20.99      C
ATOM    203  OG1 THR B 134       7.257 -55.075 -27.210  1.00 20.94      O
ATOM    204  CG2 THR B 134       6.872 -55.073 -29.600  1.00 20.64      C
ATOM    205  N   ASN B 135       9.932 -53.021 -30.075  1.00 21.24      N
ATOM    206  CA  ASN B 135      10.407 -52.419 -31.324  1.00 20.50      C
ATOM    207  C   ASN B 135      11.724 -53.064 -31.767  1.00 20.78      C
ATOM    208  O   ASN B 135      11.945 -53.290 -32.953  1.00 20.41      O
ATOM    209  CB  ASN B 135      10.637 -50.911 -31.142  1.00 19.58      C
ATOM    210  CG  ASN B 135       9.457 -50.058 -31.597  1.00 19.93      C
ATOM    211  OD1 ASN B 135       9.454 -48.837 -31.390  1.00 21.78      O
ATOM    212  ND2 ASN B 135       8.467 -50.677 -32.219  1.00 17.21      N
ATOM    213  N   LEU B 138      10.741 -56.381 -33.386  1.00 21.61      N
ATOM    214  CA  LEU B 138       9.744 -56.188 -34.431  1.00 23.15      C
ATOM    215  C   LEU B 138      10.384 -55.558 -35.676  1.00 23.07      C
ATOM    216  O   LEU B 138       9.958 -55.801 -36.809  1.00 22.68      O
ATOM    217  CB  LEU B 138       8.618 -55.305 -33.886  1.00 23.87      C
ATOM    218  CG  LEU B 138       7.312 -55.155 -34.664  1.00 26.48      C
ATOM    219  CD1 LEU B 138       6.672 -56.508 -34.915  1.00 25.34      C
ATOM    220  CD2 LEU B 138       6.383 -54.267 -33.851  1.00 25.90      C
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TABLE 6 ATOMIC COORDINATES OF MEMBRANE ASSOCIATION SITE

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REMARK    4 1MUR COMPLIES WITH FORMAT V. 2.0, 11-MAY-2000
ATOM      1  N   MET B  12      -0.734 -48.902 -33.817  1.00 23.68      N
ATOM      2  CA  MET B  12      -0.523 -49.707 -32.613  1.00 24.54      C
ATOM      3  C   MET B  12       0.361 -48.840 -31.720  1.00 25.31      C
ATOM      4  O   MET B  12       1.546 -48.645 -32.006  1.00 23.88      O
ATOM      5  CB  MET B  12       0.192 -51.019 -32.971  1.00 24.28      C
ATOM      6  CG  MET B  12      -0.402 -51.726 -34.188  1.00 25.19      C
ATOM      7  SD  MET B  12       0.399 -53.284 -34.669  1.00 26.54      S
ATOM      8  CE  MET B  12       1.990 -52.691 -35.289  1.00 22.99      C
ATOM      9  N   LEU B  40      -5.323 -50.004 -32.549  1.00 25.21      N
ATOM     10  CA  LEU B  40      -5.200 -51.364 -32.026  1.00 24.71      C
ATOM     11  C   LEU B  40      -4.535 -51.235 -30.655  1.00 23.33      C
ATOM     12  O   LEU B  40      -3.387 -50.824 -30.563  1.00 23.43      O
ATOM     13  CB  LEU B  40      -4.326 -52.221 -32.952  1.00 25.21      C
ATOM     14  CG  LEU B  40      -4.416 -53.754 -32.868  1.00 26.95      C
ATOM     15  CD1 LEU B  40      -3.037 -54.334 -32.571  1.00 27.63      C
ATOM     16  CD2 LEU B  40      -5.421 -54.179 -31.817  1.00 26.69      C
ATOM     17  N   ILE B  61      -7.271 -56.229 -28.295  1.00 29.38      N
ATOM     18  CA  ILE B  61      -6.832 -57.616 -28.269  1.00 28.55      C
ATOM     19  C   ILE B  61      -6.344 -57.855 -26.848  1.00 29.13      C
ATOM     20  O   ILE B  61      -6.124 -56.906 -26.091  1.00 28.80      O
ATOM     21  CB  ILE B  61      -5.674 -57.923 -29.258  1.00 28.48      C
ATOM     22  CG1 ILE B  61      -4.422 -57.126 -28.892  1.00 26.70      C
ATOM     23  CG2 ILE B  61      -6.123 -57.650 -30.694  1.00 27.65      C
ATOM     24  CD1 ILE B  61      -3.177 -57.615 -29.638  1.00 27.03      C
ATOM     25  N   ARG B  62      -6.186 -59.116 -26.473  1.00 29.38      N
ATOM     26  CA  ARG B  62      -5.709 -59.416 -25.133  1.00 30.76      C
ATOM     27  C   ARG B  62      -4.274 -59.923 -25.156  1.00 29.32      C
ATOM     28  O   ARG B  62      -3.933 -60.809 -25.934  1.00 28.65      O
ATOM     29  CB  ARG B  62      -6.630 -60.447 -24.461  1.00 32.36      C
ATOM     30  CG  ARG B  62      -6.130 -60.955 -23.114  1.00 35.99      C
ATOM     31  CD  ARG B  62      -5.438 -59.859 -22.311  1.00 37.86      C
ATOM     32  NE  ARG B  62      -6.297 -58.718 -22.004  1.00 40.01      N
ATOM     33  CZ  ARG B  62      -5.840 -57.504 -21.711  1.00 39.09      C
ATOM     34  NH1 ARG B  62      -4.536 -57.275 -21.690  1.00 39.24      N
ATOM     35  NH2 ARG B  62      -6.686 -56.518 -21.439  1.00 40.03      N
ATOM     36  N   ILE B  63      -3.428 -59.342 -24.313  1.00 30.07      N
ATOM     37  CA  ILE B  63      -2.036 -59.770 -24.231  1.00 31.38      C
ATOM     38  C   ILE B  63      -1.623 -59.981 -22.775  1.00 33.08      C
ATOM     39  O   ILE B  63      -0.444 -59.872 -22.430  1.00 33.21      O
ATOM     40  CB  ILE B  63      -1.081 -58.745 -24.883  1.00 30.06      C
ATOM     41  CG1 ILE B  63      -1.143 -57.411 -24.137  1.00 29.94      C
ATOM     42  CG2 ILE B  63      -1.442 -58.567 -26.353  1.00 30.41      C
ATOM     43  CD1 ILE B  63      -0.128 -56.384 -24.632  1.00 29.62      C
ATOM     44  N   SER B  64      -2.603 -60.284 -21.927  1.00 35.38      N
ATOM     45  CA  SER B  64      -2.356 -60.520 -20.505  1.00 37.51      C
ATOM     46  C   SER B  64      -1.326 -61.622 -20.311  1.00 37.32      C
ATOM     47  O   SER B  64      -1.411 -62.682 -20.933  1.00 37.86      O
ATOM     48  CB  SER B  64      -3.652 -60.912 -19.792  1.00 38.82      C
ATOM     49  OG  SER B  64      -4.558 -59.823 -19.750  1.00 42.88      O
ATOM     50  N   GLY B  65      -0.356 -61.370 -19.441  1.00 37.81      N
ATOM     51  CA  GLY B  65       0.679 -62.355 -19.199  1.00 37.13      C
ATOM     52  C   GLY B  65       1.798 -62.283 -20.226  1.00 36.76      C
ATOM     53  O   GLY B  65       2.858 -62.889 -20.038  1.00 37.57      O
ATOM     54  N   LEU B  66       1.577 -61.539 -21.307  1.00 34.63      N
ATOM     55  CA  LEU B  66       2.591 -61.413 -22.355  1.00 33.17      C
ATOM     56  C   LEU B  66       3.414 -60.133 -22.246  1.00 32.72      C
ATOM     57  O   LEU B  66       4.451 -60.002 -22.893  1.00 33.13      O
ATOM     58  CB  LEU B  66       1.936 -61.470 -23.735  1.00 32.08      C
ATOM     59  CG  LEU B  66       1.162 -62.747 -24.061  1.00 32.52      C
ATOM     60  CD1 LEU B  66       0.563 -62.626 -25.445  1.00 31.38      C
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ATOM	61	CD2	LEU	B	66	2.093	-63.957	-23.984	1.00	31.67	C
ATOM	62	N	ARG	B	67	2.953	-59.185	-21.440	1.00	31.54	N
ATOM	63	CA	ARG	B	67	3.671	-57.928	-21.277	1.00	30.90	C
ATOM	64	C	ARG	B	67	5.071	-58.142	-20.713	1.00	29.99	C
ATOM	65	O	ARG	B	67	5.294	-59.034	-19.889	1.00	28.67	O
ATOM	66	CB	ARG	B	67	2.888	-56.984	-20.363	1.00	32.28	C
ATOM	67	CG	ARG	B	67	1.540	-56.576	-20.913	1.00	34.65	C
ATOM	68	CD	ARG	B	67	0.926	-55.440	-20.097	1.00	36.69	C
ATOM	69	NE	ARG	B	67	-0.259	-54.889	-20.748	1.00	38.28	N
ATOM	70	CZ	ARG	B	67	-1.425	-55.519	-20.853	1.00	39.05	C
ATOM	71	NH1	ARG	B	67	-1.583	-56.734	-20.341	1.00	39.61	N
ATOM	72	NH2	ARG	B	67	-2.434	-54.935	-21.487	1.00	39.52	N
ATOM	73	N	GLY	B	68	6.014	-57.321	-21.165	1.00	27.75	N
ATOM	74	CA	GLY	B	68	7.380	-57.427	-20.685	1.00	26.79	C
ATOM	75	C	GLY	B	68	8.166	-58.579	-21.280	1.00	25.41	C
ATOM	76	O	GLY	B	68	9.326	-58.779	-20.943	1.00	26.04	O
ATOM	77	N	LYS	B	69	7.546	-59.342	-22.170	1.00	24.55	N
ATOM	78	CA	LYS	B	69	8.238	-60.463	-22.796	1.00	23.93	C
ATOM	79	C	LYS	B	69	8.825	-60.062	-24.142	1.00	23.32	C
ATOM	80	O	LYS	B	69	8.151	-59.404	-24.944	1.00	21.96	O
ATOM	81	CB	LYS	B	69	7.284	-61.641	-23.033	1.00	24.12	C
ATOM	82	CG	LYS	B	69	6.757	-62.360	-21.794	1.00	25.08	C
ATOM	83	CD	LYS	B	69	5.887	-63.553	-22.224	1.00	25.44	C
ATOM	84	CE	LYS	B	69	5.357	-64.358	-21.035	1.00	28.31	C
ATOM	85	NZ	LYS	B	69	6.468	-64.877	-20.175	1.00	29.71	N
ATOM	86	N	GLY	B	70	10.075	-60.470	-24.374	1.00	22.48	N
ATOM	87	CA	GLY	B	70	10.755	-60.229	-25.636	1.00	22.26	C
ATOM	88	C	GLY	B	70	10.308	-61.337	-26.588	1.00	22.17	C
ATOM	89	O	GLY	B	70	9.512	-62.183	-26.195	1.00	21.62	O
ATOM	90	N	ILE	B	71	10.819	-61.373	-27.814	1.00	21.85	N
ATOM	91	CA	ILE	B	71	10.357	-62.386	-28.762	1.00	23.55	C
ATOM	92	C	ILE	B	71	10.616	-63.840	-28.359	1.00	23.88	C
ATOM	93	O	ILE	B	71	9.775	-64.707	-28.592	1.00	21.66	O
ATOM	94	CB	ILE	B	71	10.926	-62.142	-30.181	1.00	23.52	C
ATOM	95	CG1	ILE	B	71	10.264	-63.096	-31.182	1.00	24.18	C
ATOM	96	CG2	ILE	B	71	12.435	-62.375	-30.192	1.00	25.96	C
ATOM	97	CD1	ILE	B	71	8.745	-62.981	-31.263	1.00	25.73	C
ATOM	98	N	LYS	B	72	11.764	-64.119	-27.751	1.00	23.82	N
ATOM	99	CA	LYS	B	72	12.038	-65.491	-27.343	1.00	24.92	C
ATOM	100	C	LYS	B	72	11.068	-65.925	-26.245	1.00	23.73	C
ATOM	101	O	LYS	B	72	10.592	-67.062	-26.245	1.00	24.08	O
ATOM	102	CB	LYS	B	72	13.491	-65.634	-26.875	1.00	26.86	C
ATOM	103	CG	LYS	B	72	14.496	-65.590	-28.019	1.00	31.29	C
ATOM	104	CD	LYS	B	72	15.925	-65.791	-27.518	1.00	36.00	C
ATOM	105	CE	LYS	B	72	16.926	-65.816	-28.671	1.00	38.82	C
ATOM	106	NZ	LYS	B	72	18.342	-65.957	-28.192	1.00	41.21	N
ATOM	107	N	ALA	B	73	10.765	-65.016	-25.322	1.00	21.62	N
ATOM	108	CA	ALA	B	73	9.839	-65.306	-24.233	1.00	21.18	C
ATOM	109	C	ALA	B	73	8.412	-65.454	-24.771	1.00	20.36	C
ATOM	110	O	ALA	B	73	7.619	-66.250	-24.267	1.00	18.97	O
ATOM	111	CB	ALA	B	73	9.895	-64.196	-23.187	1.00	22.25	C
ATOM	112	N	LEU	B	74	8.076	-64.673	-25.791	1.00	20.23	N
ATOM	113	CA	LEU	B	74	6.745	-64.762	-26.387	1.00	19.36	C
ATOM	114	C	LEU	B	74	6.549	-66.110	-27.069	1.00	19.37	C
ATOM	115	O	LEU	B	74	5.539	-66.779	-26.863	1.00	20.01	O
ATOM	116	CB	LEU	B	74	6.540	-63.643	-27.417	1.00	18.42	C
ATOM	117	CG	LEU	B	74	6.422	-62.208	-26.884	1.00	18.80	C
ATOM	118	CD1	LEU	B	74	6.473	-61.197	-28.039	1.00	19.86	C
ATOM	119	CD2	LEU	B	74	5.109	-62.071	-26.104	1.00	19.45	C
ATOM	120	N	ILE	B	75	7.520	-66.507	-27.883	1.00	20.59	N
ATOM	121	CA	ILE	B	75	7.434	-67.768	-28.601	1.00	21.18	C
ATOM	122	C	ILE	B	75	7.488	-68.942	-27.624	1.00	21.20	C
ATOM	123	O	ILE	B	75	7.125	-70.063	-27.979	1.00	21.59	O
ATOM	124	CB	ILE	B	75	8.571	-67.896	-29.641	1.00	22.95	C
ATOM	125	CG1	ILE	B	75	8.598	-66.657	-30.540	1.00	26.82	C
ATOM	126	CG2	ILE	B	75	8.334	-69.108	-30.527	1.00	25.38	C

ATOM	127	CD1	ILE	B	75	7.301	-66.442	-31.327	1.00	28.48	C
ATOM	128	N	ALA	B	76	7.940	-68.660	-26.399	1.00	20.49	N
ATOM	129	CA	ALA	B	76	7.996	-69.726	-25.374	1.00	21.72	C
ATOM	130	C	ALA	B	76	6.624	-69.904	-24.732	1.00	21.54	C
ATOM	131	O	ALA	B	76	6.441	-70.778	-23.875	1.00	20.75	O
ATOM	132	CB	ALA	B	76	9.026	-69.372	-24.305	1.00	21.92	C
ATOM	133	N	ALA	B	77	5.668	-69.066	-25.145	1.00	20.61	N
ATOM	134	CA	ALA	B	77	4.289	-69.121	-24.655	1.00	21.07	C
ATOM	135	C	ALA	B	77	3.383	-69.298	-25.881	1.00	21.69	C
ATOM	136	O	ALA	B	77	2.567	-68.430	-26.199	1.00	21.93	O
ATOM	137	CB	ALA	B	77	3.937	-67.830	-23.924	1.00	20.10	C
ATOM	138	N	PRO	B	78	3.507	-70.446	-26.564	1.00	22.38	N
ATOM	139	CA	PRO	B	78	2.772	-70.846	-27.771	1.00	20.95	C
ATOM	140	C	PRO	B	78	1.278	-70.535	-27.813	1.00	21.19	C
ATOM	141	O	PRO	B	78	0.789	-69.939	-28.776	1.00	19.68	O
ATOM	142	CB	PRO	B	78	3.027	-72.350	-27.861	1.00	22.21	C
ATOM	143	CG	PRO	B	78	4.288	-72.547	-27.117	1.00	24.07	C
ATOM	144	CD	PRO	B	78	4.211	-71.603	-25.976	1.00	21.89	C
ATOM	145	N	LEU	B	79	0.544	-70.961	-26.790	1.00	21.21	N
ATOM	146	CA	LEU	B	79	-0.896	-70.728	-26.783	1.00	21.32	C
ATOM	147	C	LEU	B	79	-1.275	-69.263	-26.707	1.00	21.17	C
ATOM	148	O	LEU	B	79	-2.125	-68.800	-27.481	1.00	20.44	O
ATOM	149	CB	LEU	B	79	-1.569	-71.476	-25.630	1.00	20.99	C
ATOM	150	CG	LEU	B	79	-1.397	-72.988	-25.617	1.00	22.40	C
ATOM	151	CD1	LEU	B	79	-2.504	-73.619	-24.772	1.00	22.01	C
ATOM	152	CD2	LEU	B	79	-1.438	-73.521	-27.021	1.00	23.82	C
ATOM	153	N	ARG	B	80	-0.656	-68.529	-25.788	1.00	20.91	N
ATOM	154	CA	ARG	B	80	-0.980	-67.115	-25.637	1.00	21.30	C
ATOM	155	C	ARG	B	80	-0.526	-66.233	-26.790	1.00	21.29	C
ATOM	156	O	ARG	B	80	-1.278	-65.355	-27.223	1.00	21.47	O
ATOM	157	CB	ARG	B	80	-0.444	-66.583	-24.312	1.00	22.12	C
ATOM	158	CG	ARG	B	80	-1.286	-67.051	-23.118	1.00	24.03	C
ATOM	159	CD	ARG	B	80	-0.610	-66.738	-21.807	1.00	23.42	C
ATOM	160	NE	ARG	B	80	0.581	-67.556	-21.610	1.00	24.59	N
ATOM	161	CZ	ARG	B	80	1.466	-67.351	-20.642	1.00	26.08	C
ATOM	162	NH1	ARG	B	80	1.290	-66.349	-19.787	1.00	26.92	N
ATOM	163	NH2	ARG	B	80	2.514	-68.152	-20.519	1.00	27.22	N
ATOM	164	N	ILE	B	81	0.683	-66.448	-27.303	1.00	19.29	N
ATOM	165	CA	ILE	B	81	1.113	-65.621	-28.421	1.00	19.47	C
ATOM	166	C	ILE	B	81	0.256	-65.937	-29.654	1.00	18.99	C
ATOM	167	O	ILE	B	81	-0.149	-65.028	-30.378	1.00	19.38	O
ATOM	168	CB	ILE	B	81	2.639	-65.793	-28.730	1.00	17.92	C
ATOM	169	CG1	ILE	B	81	3.067	-64.753	-29.769	1.00	18.63	C
ATOM	170	CG2	ILE	B	81	2.949	-67.200	-29.206	1.00	17.33	C
ATOM	171	CD1	ILE	B	81	2.746	-63.318	-29.346	1.00	17.46	C
ATOM	172	N	PHE	B	82	-0.056	-67.211	-29.880	1.00	19.39	N
ATOM	173	CA	PHE	B	82	-0.875	-67.582	-31.038	1.00	19.15	C
ATOM	174	C	PHE	B	82	-2.250	-66.931	-30.959	1.00	19.94	C
ATOM	175	O	PHE	B	82	-2.777	-66.444	-31.970	1.00	19.64	O
ATOM	176	CB	PHE	B	82	-1.057	-69.103	-31.136	1.00	19.27	C
ATOM	177	CG	PHE	B	82	-1.811	-69.548	-32.368	1.00	19.87	C
ATOM	178	CD1	PHE	B	82	-1.180	-69.602	-33.603	1.00	20.87	C
ATOM	179	CD2	PHE	B	82	-3.154	-69.898	-32.289	1.00	21.11	C
ATOM	180	CE1	PHE	B	82	-1.872	-70.002	-34.753	1.00	21.20	C
ATOM	181	CE2	PHE	B	82	-3.857	-70.297	-33.429	1.00	22.26	C
ATOM	182	CZ	PHE	B	82	-3.212	-70.349	-34.663	1.00	22.14	C
ATOM	183	N	ASN	B	83	-2.832	-66.923	-29.764	1.00	19.29	N
ATOM	184	CA	ASN	B	83	-4.150	-66.332	-29.577	1.00	20.90	C
ATOM	185	C	ASN	B	83	-4.178	-64.821	-29.812	1.00	20.83	C
ATOM	186	O	ASN	B	83	-5.086	-64.316	-30.472	1.00	21.92	O
ATOM	187	CB	ASN	B	83	-4.693	-66.641	-28.178	1.00	20.55	C
ATOM	188	CG	ASN	B	83	-6.158	-66.244	-28.028	1.00	22.79	C
ATOM	189	OD1	ASN	B	83	-6.505	-65.374	-27.229	1.00	25.14	O
ATOM	190	ND2	ASN	B	83	-7.018	-66.877	-28.807	1.00	20.47	N
ATOM	191	N	ALA	B	84	-3.203	-64.092	-29.275	1.00	19.74	N
ATOM	192	CA	ALA	B	84	-3.177	-62.647	-29.484	1.00	19.30	C

ATOM	193	C	ALA	B	84	-2.967	-62.380	-30.981	1.00	19.94	C
ATOM	194	O	ALA	B	84	-3.561	-61.459	-31.552	1.00	19.69	O
ATOM	195	CB	ALA	B	84	-2.060	-62.008	-28.662	1.00	18.59	C
ATOM	196	N	TRP	B	85	-2.118	-63.197	-31.603	1.00	19.77	N
ATOM	197	CA	TRP	B	85	-1.820	-63.111	-33.032	1.00	20.56	C
ATOM	198	C	TRP	B	85	-3.090	-63.354	-33.865	1.00	21.76	C
ATOM	199	O	TRP	B	85	-3.339	-62.658	-34.859	1.00	20.40	O
ATOM	200	CB	TRP	B	85	-0.754	-64.148	-33.396	1.00	21.46	C
ATOM	201	CG	TRP	B	85	-0.365	-64.167	-34.856	1.00	23.00	C
ATOM	202	CD1	TRP	B	85	0.301	-63.189	-35.548	1.00	23.17	C
ATOM	203	CD2	TRP	B	85	-0.588	-65.232	-35.785	1.00	23.69	C
ATOM	204	NE1	TRP	B	85	0.509	-63.585	-36.848	1.00	24.28	N
ATOM	205	CE2	TRP	B	85	-0.024	-64.835	-37.022	1.00	24.14	C
ATOM	206	CE3	TRP	B	85	-1.206	-66.486	-35.693	1.00	24.79	C
ATOM	207	CZ2	TRP	B	85	-0.060	-65.650	-38.160	1.00	24.90	C
ATOM	208	CZ3	TRP	B	85	-1.243	-67.299	-36.827	1.00	25.45	C
ATOM	209	CH2	TRP	B	85	-0.671	-66.875	-38.045	1.00	25.15	C
ATOM	210	N	ARG	B	86	-3.885	-64.346	-33.467	1.00	22.03	N
ATOM	211	CA	ARG	B	86	-5.140	-64.660	-34.166	1.00	23.28	C
ATOM	212	C	ARG	B	86	-6.151	-63.517	-34.007	1.00	22.98	C
ATOM	213	O	ARG	B	86	-6.890	-63.195	-34.942	1.00	21.37	O
ATOM	214	CB	ARG	B	86	-5.754	-65.965	-33.623	1.00	24.72	C
ATOM	215	CG	ARG	B	86	-4.999	-67.236	-34.021	1.00	27.21	C
ATOM	216	CD	ARG	B	86	-5.368	-67.725	-35.418	1.00	29.60	C
ATOM	217	NE	ARG	B	86	-6.626	-68.477	-35.422	1.00	31.45	N
ATOM	218	CZ	ARG	B	86	-7.185	-69.004	-36.508	1.00	31.37	C
ATOM	219	NH1	ARG	B	86	-6.607	-68.862	-37.696	1.00	32.19	N
ATOM	220	NH2	ARG	B	86	-8.314	-69.694	-36.405	1.00	31.39	N
ATOM	221	N	GLN	B	87	-6.190	-62.916	-32.821	1.00	22.90	N
ATOM	222	CA	GLN	B	87	-7.101	-61.802	-32.567	1.00	24.07	C
ATOM	223	C	GLN	B	87	-6.738	-60.618	-33.457	1.00	23.85	C
ATOM	224	O	GLN	B	87	-7.613	-60.012	-34.077	1.00	24.02	O
ATOM	225	CB	GLN	B	87	-7.046	-61.382	-31.097	1.00	24.33	C
ATOM	226	CG	GLN	B	87	-7.873	-62.280	-30.187	1.00	27.24	C
ATOM	227	CD	GLN	B	87	-7.720	-61.943	-28.723	1.00	28.81	C
ATOM	228	OE1	GLN	B	87	-8.567	-62.296	-27.908	1.00	33.25	O
ATOM	229	NE2	GLN	B	87	-6.632	-61.275	-28.375	1.00	29.95	N
ATOM	230	N	ALA	B	88	-5.449	-60.293	-33.521	1.00	23.39	N
ATOM	231	CA	ALA	B	88	-4.996	-59.183	-34.355	1.00	23.78	C
ATOM	232	C	ALA	B	88	-5.257	-59.485	-35.831	1.00	24.73	C
ATOM	233	O	ALA	B	88	-5.655	-58.595	-36.592	1.00	24.72	O
ATOM	234	CB	ALA	B	88	-3.508	-58.909	-34.116	1.00	23.33	C
ATOM	235	N	ARG	B	89	-5.038	-60.735	-36.244	1.00	24.26	N
ATOM	236	CA	ARG	B	89	-5.285	-61.111	-37.636	1.00	24.94	C
ATOM	237	C	ARG	B	89	-6.752	-60.909	-38.013	1.00	25.29	C
ATOM	238	O	ARG	B	89	-7.056	-60.420	-39.104	1.00	24.27	O
ATOM	239	CB	ARG	B	89	-4.904	-62.575	-37.893	1.00	25.14	C
ATOM	240	CG	ARG	B	89	-3.461	-62.774	-38.353	1.00	24.54	C
ATOM	241	CD	ARG	B	89	-3.142	-64.253	-38.510	1.00	25.50	C
ATOM	242	NE	ARG	B	89	-3.809	-64.901	-39.641	1.00	24.93	N
ATOM	243	CZ	ARG	B	89	-3.329	-64.930	-40.882	1.00	25.90	C
ATOM	244	NH1	ARG	B	89	-2.178	-64.336	-41.170	1.00	25.98	N
ATOM	245	NH2	ARG	B	89	-3.979	-65.596	-41.831	1.00	26.36	N
ATOM	246	N	GLY	B	105	5.583	-50.364	-27.741	1.00	23.01	N
ATOM	247	CA	GLY	B	105	4.593	-50.905	-26.827	1.00	23.54	C
ATOM	248	C	GLY	B	105	4.358	-52.380	-27.078	1.00	23.17	C
ATOM	249	O	GLY	B	105	4.449	-52.844	-28.214	1.00	22.69	O
ATOM	250	N	TYR	B	106	4.018	-53.118	-26.026	1.00	22.87	N
ATOM	251	CA	TYR	B	106	3.818	-54.554	-26.159	1.00	22.37	C
ATOM	252	C	TYR	B	106	2.719	-55.018	-27.100	1.00	20.52	C
ATOM	253	O	TYR	B	106	2.867	-56.052	-27.746	1.00	20.50	O
ATOM	254	CB	TYR	B	106	3.632	-55.181	-24.774	1.00	25.08	C
ATOM	255	CG	TYR	B	106	4.864	-55.008	-23.929	1.00	28.19	C
ATOM	256	CD1	TYR	B	106	4.869	-54.153	-22.830	1.00	31.96	C
ATOM	257	CD2	TYR	B	106	6.058	-55.631	-24.282	1.00	31.27	C
ATOM	258	CE1	TYR	B	106	6.043	-53.915	-22.108	1.00	33.13	C

ATOM	259	CE2	TYR	B	106	7.234	-55.400	-23.569	1.00	32.27	C
ATOM	260	CZ	TYR	B	106	7.219	-54.544	-22.487	1.00	33.19	C
ATOM	261	OH	TYR	B	106	8.388	-54.291	-21.802	1.00	35.95	O
ATOM	262	N	VAL	B	107	1.628	-54.270	-27.205	1.00	19.06	N
ATOM	263	CA	VAL	B	107	0.557	-54.694	-28.099	1.00	18.06	C
ATOM	264	C	VAL	B	107	1.015	-54.743	-29.559	1.00	17.45	C
ATOM	265	O	VAL	B	107	0.502	-55.536	-30.346	1.00	16.99	O
ATOM	266	CB	VAL	B	107	-0.690	-53.774	-27.978	1.00	20.95	C
ATOM	267	CG1	VAL	B	107	-0.407	-52.407	-28.589	1.00	21.39	C
ATOM	268	CG2	VAL	B	107	-1.879	-54.433	-28.658	1.00	21.30	C
ATOM	269	N	SER	B	108	1.991	-53.916	-29.918	1.00	17.96	N
ATOM	270	CA	SER	B	108	2.488	-53.892	-31.290	1.00	19.67	C
ATOM	271	C	SER	B	108	3.197	-55.187	-31.694	1.00	20.38	C
ATOM	272	O	SER	B	108	3.385	-55.449	-32.884	1.00	21.25	O
ATOM	273	CB	SER	B	108	3.424	-52.691	-31.508	1.00	19.56	C
ATOM	274	OG	SER	B	108	4.666	-52.824	-30.837	1.00	19.63	O
ATOM	275	N	GLY	B	109	3.595	-55.995	-30.710	1.00	19.59	N
ATOM	276	CA	GLY	B	109	4.251	-57.256	-31.023	1.00	20.03	C
ATOM	277	C	GLY	B	109	3.311	-58.170	-31.792	1.00	19.61	C
ATOM	278	O	GLY	B	109	3.579	-58.517	-32.940	1.00	19.24	O
ATOM	279	N	PRO	B	110	2.206	-58.606	-31.173	1.00	19.20	N
ATOM	280	CA	PRO	B	110	1.251	-59.478	-31.855	1.00	18.99	C
ATOM	281	C	PRO	B	110	0.651	-58.761	-33.075	1.00	19.22	C
ATOM	282	O	PRO	B	110	0.406	-59.371	-34.116	1.00	17.13	O
ATOM	283	CB	PRO	B	110	0.198	-59.737	-30.778	1.00	20.41	C
ATOM	284	CG	PRO	B	110	0.998	-59.720	-29.515	1.00	19.81	C
ATOM	285	CD	PRO	B	110	1.914	-58.528	-29.729	1.00	19.94	C
ATOM	286	N	GLY	B	111	0.407	-57.462	-32.927	1.00	19.03	N
ATOM	287	CA	GLY	B	111	-0.160	-56.702	-34.025	1.00	19.60	C
ATOM	288	C	GLY	B	111	0.764	-56.714	-35.226	1.00	19.59	C
ATOM	289	O	GLY	B	111	0.330	-56.979	-36.339	1.00	21.10	O
ATOM	290	N	GLY	B	112	2.043	-56.429	-34.995	1.00	19.78	N
ATOM	291	CA	GLY	B	112	3.014	-56.417	-36.074	1.00	19.97	C
ATOM	292	C	GLY	B	112	3.147	-57.783	-36.724	1.00	20.43	C
ATOM	293	O	GLY	B	112	3.233	-57.896	-37.949	1.00	19.94	O
ATOM	294	N	LEU	B	113	3.167	-58.828	-35.903	1.00	19.26	N
ATOM	295	CA	LEU	B	113	3.265	-60.184	-36.429	1.00	19.49	C
ATOM	296	C	LEU	B	113	2.040	-60.521	-37.274	1.00	18.73	C
ATOM	297	O	LEU	B	113	2.143	-61.252	-38.255	1.00	18.44	O
ATOM	298	CB	LEU	B	113	3.405	-61.198	-35.289	1.00	18.38	C
ATOM	299	CG	LEU	B	113	4.777	-61.270	-34.605	1.00	20.59	C
ATOM	300	CD1	LEU	B	113	4.656	-62.059	-33.311	1.00	20.01	C
ATOM	301	CD2	LEU	B	113	5.794	-61.914	-35.538	1.00	20.23	C
ATOM	302	N	ALA	B	114	0.875	-60.010	-36.892	1.00	18.96	N
ATOM	303	CA	ALA	B	114	-0.334	-60.292	-37.661	1.00	18.70	C
ATOM	304	C	ALA	B	114	-0.288	-59.578	-39.019	1.00	19.30	C
ATOM	305	O	ALA	B	114	-0.602	-60.167	-40.052	1.00	20.62	O
ATOM	306	CB	ALA	B	114	-1.562	-59.855	-36.889	1.00	16.45	C
ATOM	307	N	ALA	B	115	0.082	-58.303	-39.000	1.00	20.57	N
ATOM	308	CA	ALA	B	115	0.167	-57.516	-40.229	1.00	21.84	C
ATOM	309	C	ALA	B	115	1.140	-58.192	-41.189	1.00	21.58	C
ATOM	310	O	ALA	B	115	0.815	-58.464	-42.345	1.00	22.14	O
ATOM	311	CB	ALA	B	115	0.636	-56.108	-39.911	1.00	19.85	C
ATOM	312	N	TRP	B	116	2.334	-58.476	-40.688	1.00	22.12	N
ATOM	313	CA	TRP	B	116	3.365	-59.126	-41.478	1.00	23.22	C
ATOM	314	C	TRP	B	116	2.871	-60.434	-42.123	1.00	23.55	C
ATOM	315	O	TRP	B	116	3.048	-60.643	-43.329	1.00	22.19	O
ATOM	316	CB	TRP	B	116	4.584	-59.367	-40.579	1.00	26.08	C
ATOM	317	CG	TRP	B	116	5.699	-60.136	-41.204	1.00	27.40	C
ATOM	318	CD1	TRP	B	116	6.473	-59.761	-42.271	1.00	28.30	C
ATOM	319	CD2	TRP	B	116	6.168	-61.418	-40.793	1.00	28.77	C
ATOM	320	NE1	TRP	B	116	7.401	-60.742	-42.547	1.00	29.04	N
ATOM	321	CE2	TRP	B	116	7.234	-61.771	-41.655	1.00	30.37	C
ATOM	322	CE3	TRP	B	116	5.794	-62.308	-39.778	1.00	30.49	C
ATOM	323	CZ2	TRP	B	116	7.929	-62.981	-41.529	1.00	31.08	C
ATOM	324	CZ3	TRP	B	116	6.485	-63.510	-39.653	1.00	31.85	C

ATOM	325	CH2	TRP	B	116	7.541	-63.834	-40.527	1.00	32.27	C
ATOM	326	N	SER	B	117	2.231	-61.304	-41.338	1.00	21.35	N
ATOM	327	CA	SER	B	117	1.735	-62.573	-41.873	1.00	22.61	C
ATOM	328	C	SER	B	117	0.665	-62.383	-42.940	1.00	23.56	C
ATOM	329	O	SER	B	117	0.463	-63.262	-43.780	1.00	23.11	O
ATOM	330	CB	SER	B	117	1.167	-63.462	-40.756	1.00	20.72	C
ATOM	331	OG	SER	B	117	0.010	-62.889	-40.169	1.00	22.72	O
ATOM	332	N	LEU	B	133	11.788	-52.846	-25.860	1.00	23.38	N
ATOM	333	CA	LEU	B	133	11.903	-54.293	-26.020	1.00	24.54	C
ATOM	334	C	LEU	B	133	11.209	-54.833	-27.276	1.00	22.84	C
ATOM	335	O	LEU	B	133	11.784	-55.619	-28.027	1.00	21.86	O
ATOM	336	CB	LEU	B	133	11.328	-54.996	-24.786	1.00	25.48	C
ATOM	337	CG	LEU	B	133	11.388	-56.527	-24.780	1.00	27.50	C
ATOM	338	CD1	LEU	B	133	12.840	-56.984	-24.866	1.00	28.69	C
ATOM	339	CD2	LEU	B	133	10.735	-57.059	-23.509	1.00	28.04	C
ATOM	340	N	THR	B	134	9.975	-54.401	-27.499	1.00	21.72	N
ATOM	341	CA	THR	B	134	9.202	-54.860	-28.639	1.00	21.22	C
ATOM	342	C	THR	B	134	9.693	-54.326	-29.986	1.00	20.62	C
ATOM	343	O	THR	B	134	9.843	-55.091	-30.932	1.00	20.33	O
ATOM	344	CB	THR	B	134	7.716	-54.509	-28.449	1.00	20.99	C
ATOM	345	OG1	THR	B	134	7.257	-55.075	-27.210	1.00	20.94	O
ATOM	346	CG2	THR	B	134	6.872	-55.073	-29.600	1.00	20.64	C
ATOM	3608	N	LYS	B	136	12.595	-53.366	-30.809	1.00	21.46	N
ATOM	3609	CA	LYS	B	136	13.886	-53.949	-31.144	1.00	22.79	C
ATOM	3610	CB	LYS	B	136	14.713	-54.196	-29.879	1.00	24.70	C
ATOM	3611	CG	LYS	B	136	16.183	-54.424	-30.178	1.00	27.75	C
ATOM	3612	CD	LYS	B	136	16.998	-54.494	-28.902	1.00	30.17	C
ATOM	3613	CE	LYS	B	136	18.479	-54.671	-29.203	1.00	32.33	C
ATOM	3614	NZ	LYS	B	136	19.278	-54.641	-27.944	1.00	33.37	N
ATOM	3615	C	LYS	B	136	13.793	-55.229	-31.966	1.00	23.46	C
ATOM	3616	O	LYS	B	136	14.561	-55.407	-32.912	1.00	23.71	O
ATOM	347	N	TRP	B	137	12.868	-56.127	-31.633	1.00	21.78	N
ATOM	348	CA	TRP	B	137	12.753	-57.345	-32.424	1.00	22.06	C
ATOM	349	C	TRP	B	137	11.768	-57.202	-33.574	1.00	21.75	C
ATOM	350	O	TRP	B	137	11.936	-57.822	-34.623	1.00	21.76	O
ATOM	351	CB	TRP	B	137	12.361	-58.552	-31.553	1.00	21.20	C
ATOM	352	CG	TRP	B	137	10.990	-58.525	-30.922	1.00	20.23	C
ATOM	353	CD1	TRP	B	137	10.696	-58.231	-29.618	1.00	19.62	C
ATOM	354	CD2	TRP	B	137	9.748	-58.877	-31.544	1.00	18.68	C
ATOM	355	NE1	TRP	B	137	9.349	-58.385	-29.390	1.00	19.31	N
ATOM	356	CE2	TRP	B	137	8.743	-58.780	-30.555	1.00	18.97	C
ATOM	357	CE3	TRP	B	137	9.383	-59.270	-32.840	1.00	19.75	C
ATOM	358	CZ2	TRP	B	137	7.401	-59.058	-30.821	1.00	18.18	C
ATOM	359	CZ3	TRP	B	137	8.046	-59.549	-33.107	1.00	18.87	C
ATOM	360	CH2	TRP	B	137	7.072	-59.440	-32.099	1.00	18.94	C
ATOM	361	N	LEU	B	138	10.741	-56.381	-33.386	1.00	21.61	N
ATOM	362	CA	LEU	B	138	9.744	-56.188	-34.431	1.00	23.15	C
ATOM	363	C	LEU	B	138	10.384	-55.558	-35.676	1.00	23.07	C
ATOM	364	O	LEU	B	138	9.958	-55.801	-36.809	1.00	22.68	O
ATOM	365	CB	LEU	B	138	8.618	-55.305	-33.886	1.00	23.87	C
ATOM	366	CG	LEU	B	138	7.312	-55.155	-34.664	1.00	26.48	C
ATOM	367	CD1	LEU	B	138	6.672	-56.508	-34.915	1.00	25.34	C
ATOM	368	CD2	LEU	B	138	6.383	-54.267	-33.851	1.00	25.90	C
ATOM	3644	N	LYS	B	140	12.801	-56.332	-37.241	1.00	27.38	N
ATOM	3645	CA	LYS	B	140	13.279	-57.337	-38.182	1.00	28.05	C
ATOM	3646	CB	LYS	B	140	13.893	-58.501	-37.401	1.00	29.91	C
ATOM	3647	CG	LYS	B	140	15.134	-58.057	-36.635	1.00	31.62	C
ATOM	3648	CD	LYS	B	140	15.719	-59.149	-35.757	1.00	33.53	C
ATOM	3649	CE	LYS	B	140	16.974	-58.634	-35.055	1.00	34.46	C
ATOM	3650	NZ	LYS	B	140	17.692	-59.713	-34.320	1.00	36.17	N
ATOM	3651	C	LYS	B	140	12.254	-57.833	-39.212	1.00	27.83	C
ATOM	3652	O	LYS	B	140	12.602	-58.562	-40.142	1.00	27.80	O
ATOM	369	N	ILE	B	141	10.992	-57.445	-39.052	1.00	26.40	N
ATOM	370	CA	ILE	B	141	9.963	-57.818	-40.016	1.00	26.09	C
ATOM	371	C	ILE	B	141	9.316	-56.542	-40.530	1.00	25.81	C
ATOM	372	O	ILE	B	141	8.353	-56.586	-41.305	1.00	26.10	O

ATOM	373	CB	ILE	B	141	8.854	-58.721	-39.405	1.00	26.39	C
ATOM	374	CG1	ILE	B	141	8.298	-58.09-23-	-38.127	1.00	26.45	C
ATOM	375	CG2	ILE	B	141	9.401	-60.118	-39.145 '	1.00	28.33	C
ATOM	376	CD1	ILE	B	141	7.136	-58.845	-37.549	1~00	26.95	C
TER											

The following examples are presented for purposes of illustration only and are not intended to limit the scope of the invention in any way.

EXAMPLE I

This example describes the crystallization of the *E. coli* MurG protein and the determination of the coordinates of the three-dimensional crystal structure. This example also describes the identification of the donor nucleotide binding site, the acceptor binding site and the membrane association site of the MurG protein.

Abstract

The 1.9 Å X-ray structure of a membrane-associated glycosyltransferase involved in peptidoglycan biosynthesis is reported. This enzyme, MurG, contains two α/β open sheet domains separated by a deep cleft. The C-terminal domain contains the LTDP-GlcNAc binding site while the N-terminal domain contains the acceptor binding site and likely membrane association site. Combined with sequence data from other MurG homologs, this structure provides insight into the residues that are important in substrate binding and catalysis. We have also noted that a conserved region *found in* many UDP-sugar transferases maps to a $\beta/\alpha/\beta/\alpha$ supersecondary structural motif in the donor binding region of MurG, an observation that is be helpful in glycosyltransferase structure prediction.

Methods

Crystallization

E. coli MurG containing a C-terminal LEHHHHHH sequence was purified as described(Ha et al., 1999) and concentrated to 10 mg ml-' in 20 mM Tris-HCl, pH 7.9/ 150 mM NaCl/ 50 mM EDTA. The protein concentrate was mixed with UDP-GlcNAc in a 1:3 molar ratio. Crystals were grown at room temperature using the hanging-drop vapor-diffusion method by mixing equal volumes of protein with reservoir solution (0. 1 M NaMES, pH 6.5/ 0.96 M $(NH_4)_2SO_4$/ 0.4% Triton X-100/

10 mM DTT). Triclinic crystals with a typical size of 0.2 mm X 0.1 mm X 0.1 mm grew within a week. The crystals belong to the PI space group, with two molecules per asymmetric unit. The cell dimensions are a=60.613 Å, b=66.356 Å, c=67.902 Å, α=64.294, β=83.520, γ=65.448

Data collection and processing

All data sets were collected at 100 K on previously flash frozen crystals. Crystals were equilibrated in a cryoprotectant buffer with 0.1 M NaMES, pH 6.5, 1.44 M $(NH_4)_2SO_4$, 0.4% Triton X-100, and 20% glycerol. Heavy-atom soaks were carried out in the same buffer containing one of the following heavy-atom solutions: 2 mM $HgCl_2$, 1 mM $(NH_4)_2WS_4$, 1 mM $(NH_4)_2OsBr_6$. Crystals were flash-frozen in liquid nitrogen. HgC_2 (form A derivative) and $(NH_4)_2OsBr_6$ derivative data were collected at an R-AXISIIC imaging plate detector mounted on a Rigaku 200HB generator. Native, $HgCl_2$ (form B derivative), and $(NH_4)_2WS_4$ derivative diffraction data were collected at beam-line BioCARS-14B at the Advanced Photon Source, at wavelengths 1.0092 Å, 0.9900 Å and 1.2147 Å respectively. Collection of data on the $HgCl_2$, derivative was initially designed for MAD phasing; however, the mercury derivative proved to be unstable to X-rays, and after a two-hour exposure to synchrotron radiation the form A derivative metamorphosed into a different mercury derivative (form B) that was suitable for MIR phasing. All the data were reduced using DENZO and SCALEPACK (Otwinowski & Minor, 1997), and processed with CCP4 programs (CCP4, 1994).

Structure determination and refinement

The structure was solved by multiple isomorphous replacement combined with anomalous scattering of mercuric derivatives (Table 1). Initial MIR phases calculated with program MLPHARE had a mean figure of merit of 0.44 to 2.5 Å, and were improved by solvent flattening and histogram matching using DM. An MIR map was generated which had continuous electron density for most regions of the protein. A model was built with the program O (Jones et al., 1991), and the structure was refined against 1.9 Å data using energy minimization, simulated annealing and B-factor refinement with the program CNS (Brunger et at., 1998). The N-terminal six residues and the C-terminal His-tag had no electron density and were not included in this model. There was no electron density for UDP-GlcNAc.

Results and discussion

Overall fold

The crystal structure of E. coli MurG was solved by a combination of multiple isomorphous replacement and anomalous scattering, and refined to 1.9 Å resolution (Table 1).

TABLE 1

Summary of crystallographic and refinement data

Data set	Native	$HgCl_2$ (form A derivative)	$HgCl_2$ (form B derivative)	$(NH_4)_2WS_4$	$(NH_4)_2OsBr_6$
Resolution (Å)	1.9	2.0	1.9	2.4	2.3
Observations	288,150	101,913	245,320	44,366	106,606
Unique reflections	65,567	53,391	65,581	27,950	36,443
R_{sym}[1] (last shell)	0.032 (0.187)	0.043 (0.200)	0.042 (0.296)	0.031 (0.080)	0.056 (0.302)
I/σ (last shell)	41.9(7.0)	20.4(2.9)	29.0(3.7)	24.6(8.2)	19.6(2.5)
Completeness (last shell)	97.7% (96.4%)	91.4% (66.6%)	97.4% (94.0%)	83.8% (62.0%)	94.3% (78.6%)
MIR analysis (40.0 - 2.5 Å)					
Mean isomorphous difference[2]		0.163	0.130	0.068	0.134
Phasing power[3] (last shell)		1.09(0.73)	0.57(0.50)	0.61(0.24)	0.61(0.58)
R_{cullis} [4](last shell)		0.81 (0.91)	0.94(0.96)	0.92(0.99)	0.94(0.95)
Anomalous R_{cullis} [4](last shell)		0.96(1.00)	0.95(1.00)		
Refinement statistics					
Resolution	40.0 - 1.9 Å	R. m. s. d.[7]			
Reflections ($\|F\| > 2\sigma$)	61,989	Bonds (Å)		0.006	
Protein atoms (a. u.)	5,280	Angles(°)		1.29	
Water Atoms	298				
Sulfate groups	1	Ramachandran plot[8]			
R-factor-[5]	22.0%	Residues in most favored region		94.6%	
R-free[6]	24.7%	Residues in additional allowed region		5.4%	

[1] $R_{sym} = \Sigma|I_i - \langle I \rangle| / \Sigma I_i$, where I_i is the intensity of a reflection, and $\langle I \rangle$ is the average intensity of that reflection.
[2] Mean isomorphous difference = $\Sigma |F_{PH} - F_P| / \Sigma F_{PH}$, where F_{PH} and F_P are the derivative and native structure factors respectively.
[3] Phasing power is the ratio of the mean calculated derivative structure factor to the mean lack of closure error.
[4] R_{cullis} is the mean residual lack of closure error divided by the dispersive or anomalous difference.
[5] R-factor = $\Sigma|Fobs| - |Fcalc| | / \Sigma| F|$
[6] R-free is the R-factor calculated using 10% of the reflection data chosen randomly and omitted from the start of refinement.
[7] R. m. s. d., root-mean-square deviations from ideal bond lengths and bond angles.
[8] Calculated with program PROCHECK.

The structure consists of two domains separated by a deep cleft (Fig. 2a). Both domains exhibit an α/β open-sheet structure and have high structural homology despite minimal sequence homology (RMSD = 2.02 over 85 aligned Cα atoms). The N-domain includes residues 7-163 and 341-357, and contains seven parallel β-strands and six α -helices, the last of which originates in the C-domain (Fig. 2b). The C-domain comprises residues 164-340 and contains six parallel β-strands and eight α -helices, including one irregular bipartite helix (α-link) that connects the N-domain to the first β-strand of the C-domain. The β-strands in both domains are ordered as for a typical Rossman fold. The N- and C-domains are joined by a short linker between the seventh β-strand of the N-domain and the α-link of the C-domain. This inter-domain linker and the peptide segment that joins the last helix of the C-domain to the last helix of the N-domain define the floor of the cleft between the two domains. The cleft itself is about 20 Å deep and 18 Å across at its widest point. Contacts < 4 Å across the cleft are limited primarily to interactions between residues from C-α5 to the loop connecting N-β5 to N-α5.

The α/β open-sheet motif (Rossman fold) adopted by both the N- and C-domains of MurG is characteristic of domains that bind nucleotides (Branden & Tooze, 1998). Classical Rossman domains typically contain at least one conserved glycine rich motif, with the consensus sequence GXGXXG, located at a turn between the carboxyl end of one β-strand and the amino terminus of the adjacent α-helix (Baker et al., 1992). This motif is involved in binding the negatively charged phosphates (Carugo & Argos, 1997). There are three glycine rich loops (G loops) in *E. coli* MurG (Fig. 3a) that may be variants on the phosphate binding loops found in other dinucleotide binding proteins (see below).

Sequence homology

Amino acid sequences for eighteen MurG homologs are now available. The sequence similarity between *E. coli* MurG and homologs from other bacterial strains ranges from less than 30% to more than 90% depending on the evolutionary relationship between the organisms. In all MurG homologs, however, there are several invariant residues. Fig. 3a shows a sequence alignment for a subset of MurG homologs with the invariant and highly conserved residues indicated. These residues,

which include the three G loops, have been highlighted in the *E. coli* MurG structure (Fig. 3b). Almost all of the invariant residues are located at or near the cleft between the two domains. Two of the G loops are found in the N domain (between N-β1/N-αl and N-β4/N-α4) and one is found in the C-domain (between C-β1/C-αl). The strict conservation of the highlighted residues among different bacterial strains, and their location as determined from the *E. coli* MurG structure, implicates them in substrate binding and catalytic activity.

Structural homology reveals the donor binding site

The three-dimensional backbone structure of *E. coli* MurG was compared to known protein structures, including the three other NDP-glycosyltransferase structures that have been reported (Chamok & Davies, 1999; Gastinel *et al.,* 1999; Vrielink *et al., 1994).* The C-terminal domain was found to have significant structural homology (RMSD= 2.218 Å for 89 aligned C? atoms) to the C-terminal domain of phage T4 β-glucosyltransferase (BGT), an enzyme that catalyzes the glucosylation of hydroxymethyl-cytosines in duplex DNA. A co-crystal structure of BGT with UDP bound in the C-terminal domain reveals the topology of the UDP binding pocket and also shows important contacts to the nucleotide (Moréra *et al.,* 1999; Vrielink *et al.,* 1994). These contacts include: a) hydrogen bonds from the backbone amide of 1238 to the N3 and O4 positions of the base; b) hydrogen bonds between the carboxyl side chain of E272 and the O2' and O3' hydroxyls of the ribose ring; and c) contacts from a GGS motif in the loop following the first β-strand of the C domain to the alpha phosphate of UDP. The structurally homologous C-domain of MurG contains a topologically similar pocket (Fig. 4a). Furthermore, even though the two domains share only 11% sequence identity overall, there are identical residues in the same spatial location in *E. coli* MurG and in BGT. Based on this comparison, we have concluded that the C-domain of *E. coli* MurG is the UDP-GlcNAc binding site.

We have docked UDP-GlcNAc into the C-domain of E. coli MurG using the information on how UDP binds to BGT as a guide. As shown in Figure 4b, the uracil is held in place by contacts from the N3 and O4 atoms to the backbone amide of I245. The O2' and O3' hydroxyls on the ribose sugar are within hydrogen bonding distance of the invariant glutamate residue (E269) in the middle of helix C-?4. The conserved GGS motif in G loop 3 is positioned to contact the alpha phosphate. When these

contacts are made, the UDP-GlcNAc substrate fits nicely into a pocket in the C-domain, where it is surrounded by many of the invariant residues identified through sequence analysis of other MurG homologs. It is possible to propose roles for some of these invariant residues from the model. For example, the side chain of R261 can be rotated to contact the second phosphate; this contact may help explain why UDP binds significantly better to MurG than UMP. We propose that R261 plays an important role in catalysis by stabilizing the UDP leaving group via electrostatic interactions. The side chain of Q289 is within hydrogen bonding distance of the C4 hydroxyl of the GlcNAc sugar. This contact may explain why MurG can discriminate between UDP-GlcNAc and its C4 axial isomer, UDP-GalNAc (Ha *et at.,* 1999).

The acceptor binding site

Structural considerations suggest that the primary acceptor binding site is located in the N-terminal domain of MurG. This domain contains three highly conserved regions, two of which are glycine-rich loops that face the cleft (Fig 3a and 4c). These G loops are reminiscent of the phosphate binding loops found in other nucleotide binding proteins, and are most likely involved in binding to the diphosphate on Lipid I. The N-termini of the helices following each G loop form opposite walls of a small pocket between the G loops. The helix dipoles create a positively charged electrostatic field in the pocket that can stabilize the negative charged diphosphates. When the diphosphate of the acceptor is anchored in the pocket created by the G-loops, the MurNAc sugar emerges into the cleft between domains and the C4 hydroxyl can be directed towards the anomeric carbon of the GlcNAc for attack on the face opposite the UDP leaving group. The third conserved region in the N domain spans the loop from the end of N-?5 to the middle of N-?5. Kinetic analysis of mutants is required to evaluate the roles of these residues (Ha *et al.,* 1999; Men *et al.,* 1998).

Proposed membrane association site

MurG associates with the cytoplasmic surface of bacterial membranes where it couples a soluble donor sugar to the membrane anchored acceptor sugar, Lipid I. Analysis of the *E. coli* MurG structure shows that there is a hydrophobic patch consisting of residues I75, L79, F82, W85 and W116 in the N-domain, which is surrounded by basic residues (K72, K140, K69, R80, R86, R89). We propose that this

is the membrane association site and that association involves both hydrophobic and electrostatic interactions with the negatively charged bacterial membrane. The location of this patch in MurG is also consistent with the proposed acceptor binding site: membrane association at this patch would bring the two N-terminal G loops close to the membrane surface where the diphosphate portion of the acceptor is located (Fig. 4c). Moreover, the cleft between the two domains would remain accessible, consistent with the biochemical requirement that the soluble UDP-GlcNAc donor be able to find its binding site from the cytoplasm.

Implications for other glycosyltransferases

Glycosyltransferases that utilize an activated nucleotide sugar as a donor comprise a large family of enzymes in both prokaryotes and eukaryotes, and they play central roles in many important biological processes (Dennis *et al.*, 1999; Koya *et al.*, 1999; Verbert & Cacan, 1999). Glycosyltransferases are typically classified according to the nucleotide sugar they utilize, and it has frequently been noted that there is no significant sequence homology even among glycosyltransferases in the same family. This has made it difficult to identify common structural features and residues important in binding and catalysis. There are only three other glycosyltransferase structures available, and although none of them shows any sequence homology to MurG, a structural comparison indicates that one of them, BGT, contains a related donor binding site.

In addition to this structural homology, we have identified a strikingly similar sequence motif in the MurG family and certain other UDP-glycosyltransferase families. This sequence motif spans about a thirty amino acid stretch in the C-domain of MurG and includes most of the invariant residues found in that domain. As shown in Figure 3a, a similar motif is found in the UDP-glucuronosyltransferases (Mackenzie, 1990). Certain residues are identical, including a number of prolines and glycines, and the spacing between them is invariant. This suggests that the UDP-glucuronosyltransferases contain a region of α/β supersecondary structure that is involved in a similar function as the corresponding region in MurG (Fig. 3c). This region binds the donor sugar. By analyzing the similarities and differences between the conserved residues in this subdomain in the MurG family and other UDP-glycosyltransferase families, it may be possible to identify - and perhaps alter - residues that are involved in determining donor

selectivity. We note that it would be useful to be able to manipulate donor specificity because it would extend the utility of glycosyltransferases as reagents for glycosylation of complex molecules. Altered glycosyltransferases could also be useful for remodeling cell surfaces and for probing the biological roles of particular carbohydrate structures.

Conclusion

This first structure of a member of the MurG family of glycosyltransferases lays the groundwork for further mechanistic and structural investigations, which may lead to the design of inhibitors and perhaps even new antibiotics. The work also shows that there can be conserved subdomains even in very different glycosyltransferase families. Information on conserved subdomains will be useful for structure prediction and may help guide experiments directed towards changing substrate specificity.

EXAMPLE2

This example describes a method of isolating the C-terminal domain of the *E. coli* MurG protein, expressing the domain in *E. coli* cells and utilizing nuclear magnetic resonance (NMR) to determine the ability of compounds to bind.

MurG can also be used to determine the ability of a chemical compound to bind to the C domain by a) determining the start of c domain based on the MurG crystal structure; b) independently expressing the C domain; and c) using NMR methods to identify binding site and/or bound conformation of ligand. The same procedure is used for the acceptor binding domains.

NMR methods are used to identify the protein binding sites and screen for ligands that bind. The MurG C-terminal domain region of the protein has been expressed independently. The C domain has a much lower molecular weight than the full-length protein. Therefore, the expression of the C domain results in much sharper NMR peaks which will facilitate the NMR interpretation. Also the proton chemical shifts are very sensitive to their environment. Binding of a compound will introduce local environment changes, thus changing the proton chemical shifts. In this way, residues involved in the binding can be differentiated easily from other amino acid residues not involved in binding a ligand. This method has also been used to identify ligands that bind to low molecular weight drug targets (i.e., small proteins).

Relevant references to NMR techniques are: Discovering high-affinity ligands for proteins: SAR by NMR, S. Shuker, P. Hajduk, R. Meadows, and S. Fesik, Science 274, 1531 (1996); Lin Y, Nageswara Rao BD. Structural characterization of adenine nucleotides bound to Escherichia coli adenylate kinase. 1. Adenosineconformations by proton two-dimensional transferred nuclear Overhauser effect spectroscopy. Biochemistry. 2000 Apr 4;39(13):3636-46; and Fejzo J, et al., Chem Biol 1999 Oct,6(10):755-69 (incorporated herein by reference).

The SHAPES strategy is also useful for NMR identification of binding residues, ligands and drug discover which is an NMR-based approach for lead generation in drug discovery. Recently, it has been shown that nuclear magnetic resonance (NMR) may be used to identify ligands that bind to low molecular weight protein drugtargets. Recognizing the utility of NMR as a very sensitive method for detecting binding, we have focused on developing alternative approaches that are applicable to larger molecular weight drug targets and do not require isotopic labeling. A new method for lead generation (SHAPES) uses NMR to detect the binding of a limited but diverse library of small molecules to a potential drug target. The compound scaffolds are derived from shapes most commonly found in known therapeutic agents. NMR detection of low (microM-mM) affinity binding is achieved using either differential line broadening or transferred NOE (nuclear Overhauser effect) NMR techniques. The SHAPES method for lead generation by NMR is useful for identifying potential lead classes of drugs early in a drug design program, and is easily integrated with other discovery tools such as virtual screening, high-throughput screening and combinatorial chemistry.

EXAMPLE 3

This example describes the method of using the three-dimensional structure of *E. coli* MurG to determine the crystal structures of its mutant, enzyme-ligand complex, and MurG homologs, which share the same folding motif.

First, a crystalline form of the new protein or the protein complex should be obtained. The E.coli MurG mutants should be crystallized in a condition very similar to what we have showed in the method section. The.protein-ligand complex can be obtained by soaking the protein crystals in a ligand-containing buffer. Other MurG homologs can be expressed in a His-tagged fashion and purified using affinity colume.

Presumably they can be crystallized in a similar way using a detergent as the additive. Next, the diffraction data should be collected and processed. After the data collection, the molecular replacement method is used to determine the unknown structure. Either the whole *E. coli* MurG protein or one single domain can serve as a search model. This search model can be rotated and translated until the correct orientation is located in the unit cell of this unknown structure. The search model may only represent part of the contents of the asymmetric unit. However, the location of the first model is now already available. While the first location of the search model is fixed, the second round of translation search can be carried out to search more molecules or domains in the asymmetric unit cell. The phases from the final model generated by molecular replacement can be used to calculate the electron density map. Finally, a model is built based on the electron density map, and the model needs to be refined using program CNS or XPLOR.

EXAMPLE 4

This example describes the method of using the three-dimensional coordinate structure of *E. coli* MurG to produce a protein fragment that can be used in an NMR-based lead discovery program. The crystal structure reveals the boundaries of the C domain and permits us to design a gene containing only the C domain from the gene containing both domains. The C domain starting at residue 164 and ending at residue 340 was cloned into an expression vector to generate a C-terminal His-tag fusion, It was over-expressed in *E. coli* cells and purified by affinity colume. The protein was shown to be monomeric by size exclusion chromatography and to be soluble at least up to 0.15 mM, a concentration more than adequate for NMR analysis. C domains from other MurG homologues can be similarly expressed and used.

EXAMPLE 5

This example describes the co-crystallization of a MurG protein with a ligand. A MurG-ligand complex is formed by either co-crystallizing MurG protein with appropriate ligand or soaking the MurG crystals in buffers containing appropriate ligand. Co-crystallization is done by pre-mixing the protein sample with a certain amount of substrate or substrate analogs. Then the hanging drop method is used to produce crystals as described infra.

Alternatively, ligans are incorporated into the crystals by soaking the protein crystals in the ligand containing buffer for a period of time to allow for infiltration into the crystal. The time ranges from a couple of hours to a couple of days. The concentration of ligand in the buffer ranges from several milimolar to several hundred mili molar.

DEPOSIT OF COORDINATES

The crystal structure three-dimensional coordinates of the *E. coli* MurG as set forth in Table 1 were deposited with the Protein Data Bank and have been assigned the indicated ID Code (Accession No.) 1F0K.

Although the invention is described in detail with reference to specific embodiments thereof, it will be understood that variations which are functionally equivalent are within the scope of this invention. Indeed, various modifications of the invention in addition to those shown and described herein will become apparent to those skilled in the art from the foregoing description and accompanying drawings. Such modifications are intended to fall within the scope of the appended claims.

Various publications are cited herein, the disclosures of which are incorporated by reference in their entireties.

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WHAT IS CLAIMED IS:

1. A composition comprising the *E. coli* MurG protein in crystalline form.

2. A composition comprising a MurG protein in crystalline form.

3. A three-dimensional structure of the crystalline form of an *E. coli* MurG protein, wherein the three-dimensional structure substantially conforms to the atomic coordinates represented in Table 1.

4. A three-dimensional structure of the crystalline form of a MurG protein, wherein the three-dimensional structure substantially conforms to the atomic coordinates represented in Table 1.

5. A three-dimensional structure of the α-carbon backbone of the crystalline form of an *E. coli* MurG protein, wherein the three-dimensional structure substantially conforms to the atomic coordinates represented in Table 2.

6. A three-dimensional structure of the α-carbon backbone and conserved amino acid residues of an E coli MurG protein, wherein the three-dimensional structure substantially conforms to the atomic coordinates represented in Table 3.

7. A three-dimensional structure of a donor nucleotide binding site of a MurG protein wherein the three-dimensional structure structure of the donor nucleotide binding site substantially conforms to the atomic coordinates in Table 4.

8. The three-dimensional structure of claim 7, wherein the donor nucleotide is UDP-GlcNAc.

9. A three-dimensional structure of an acceptor binding site of a MurG protein substantially conforming to the atomic coordinates in Table 5.

10. A three-dimensional structure of a membrane association site of a MurG protein substantially conforming to the atomic coordinates in Table 6.

11. A three-dimensional computer image of the three-dimensional structure of a MurG protein.

12. The image of claim 11, wherein the structure substantially conforms with the three-dimensional coordinates listed in Table 1.

13. The image of claim 11, wherein the computer image that is generated when a set of three-dimensional coordinates comprising the three-dimensional coordinates represented in Table 1 are analyzed on a computer using a graphical display software program to create an electronic file of the image and visualizing the electronic

file on a computer capable of representing the electronic file as a three-dimensional image.

14. The image of claim 11, wherein the three-dimensional computer image is represented by a two dimensional image selected from the group consisting of Fig. 2a, 3a, or 4c.

15. The image of claim 11, wherein the three-dimensional computer image is used to design a compound.

16. A three-dimensional computer image of the three-dimensional structure of the α-carbon backbone of a MurG protein.

17. The image of claim 16, wherein the structure substantially conforms with the three-dimensional coordinates listed in Table 2.

18. The image of claim 16, wherein the computer image is that is generated when a set of three-dimensional coordinates comprising the three-dimensional coordinates represented in Table 2 are analyzed on a computer using a graphical display software program to create an electronic file of the image and visualizing the electronic file on a computer capable of representing the electronic file as a three-dimensional image.

19. The image of claim 16, wherein the three-dimensional computer image is used to design a compound.

20. A three-dimensional image of the three-dimensional image of an α-carbon backbone and conserved amino acid residues of a MurG protein.

21. The image of claim 20, wherein the structure substantially conforms with the three-dimensional coordinates in Table 3.

22. The image of claim 21, wherein the computer image is that is generated when a set of three-dimensional coordinates comprising the three-dimensional coordinates represented in Table 3 are analyzed on a computer using a graphical display software program to create an electronic file of the image and visualizing the electronic file on a computer capable of representing the electronic file as a three-dimensional imaie.

23. The image of claim 21, wherein the three-dimensional computer image is used to design a compound.

24. A three-dimensional computer image of the three-dimensional structure of a donor nucleotide binding site of a MurG protein.

25. The image of claim 24, wherein the structure substantially conforms with the three-dimensional coordinates in Table 4.

26. The image of claim 24, wherein the computer image is that is generated when a set of three-dimensional coordinates comprising the three-dimensional coordinates represented in Table 4 are analyzed on a computer using a graphical display software program to create an electronic file of the image and visualizing the electronic file on a computer capable of representing the electronic file as a three-dimensional image.

27. The image of claim 24, wherein the three-dimensional computer image is rep resented by a two dimensional image selected from the group consisting of Fig. 3c, 4a or 4b.

28. The image of claim 24, wherein the three-dimensional computer image is used to design a compound.

29. A three-dimensional computer image of the three-dimensional structure of an acceptor binding site of a MurG protein.

30. The image of claim 29, wherein the structure substantially conforms with the three-dimensional coordinates Table 5.

31. The image of claim 29, wherein the computer image is that is generated when a set of three-dimensional coordinates comprising the three-dimensional coordinates represented in Table 5 are analyzed on a computer using a graphical display software program to create an electronic file of the image and visualizing the electronic file on a computer capable of representing the electronic file as a three-dimensional image.

32. The image of claim 29, wherein the three-dimensional computer image is represented by the two dimensional image of Fig. 4a.

33. The image of claim 29, wherein the three-dimensional computer image is used to design a compound.

34. A three-dimensional computer image of the three-dimensional structure of a membrane association site of a MurG protein.

35. The image of claim 34, wherein the structure substantially conforms with the three-dimensional coordinates Table 6.

36. The image of claim 34, wherein the computer image is that is generated when a set of three-dimensional coordinates comprising the three-dimensional coordinates represented in Table 6 are analyzed on a computer using a graphical display software program to create an electronic file of the image and visualizing the electronic file on a computer capable of representing the electronic file as a three-dimensional image.

37. The image of claim 34, wherein, the three-dimensional computer image is represented by the two dimensional image of Fig. 4a.

38. The image of claim 34, wherein the three-dimensional computer image is used to design a compound.

39. A computer readable medium encoded with a set of three-dimensional coordinates of a MurG protein having a three-dimensional structure that substantially conforms to the atomic coordinates of Table 1, wherein using a graphical display software program, the three-dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three-dimensional image.

40. A computer readable medium encoded with a set of three-dimensional coordinates of an α-carbon backbone of a MurG protein having a three-dimensional structure that substantially conforms to the atomic coordinates of Table 2, wherein using a graphical display software program, the three-dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three-dimensional image.

41. A computer readable medium encoded with a set of three-dimensional coordinates of an α-carbon backbone and conserved amino acid residues of a MurG protein having a three-dimensional structure that substantially conforms to the atomic coordinates of Table 3, wherein using a graphical display software program, the three-dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three-dimensional image.

42. A computer readable medium encoded with a set of three-dimensional coordinates of a donor nucleotide binding site of a MurG protein having a three-

dimensional structure that substantially conforms to the atomic coordinates of Table 4, wherein using a graphical display software program, the three-dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three-dimensional image.

43. A computer readable medium encoded with a set of three-dimensional coordinates of an acceptor binding site of a MurG protein having a three-dimensional structure that substantially conforms to the atomic coordinates of Table 5, wherein using a graphical display software program, the three-dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three-dimensional image.

44. A computer readable medium encoded with a set of three-dimensional coordinates of a membrane association site of a MurG protein having a three-dimensional structure that substantially conforms to the atomic coordinates of Table 5, wherein using a graphical display software program, the three-dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three-dimensional image.

45. A method for identifying a potential inhibitor of a UDP-glycosyltransferase enzyme, the method comprising the steps of:

(a) using a three-dimensional structure of UDP-glycosyltransferase enzyme as defined by atomic coordinates of UDP-glycosyltransferase enzyme according to FIG. 5;

(b) employing said three-dimensional structure to design or select said potential inhibitor;

(c) synthesizing said potential inhibitor; and

(d) contacting said potential inhibitor with said UDP-glycosyltransferase enzyme in the presence of a substrate to test the ability of said potential inhibitor to inhibit said UDPglycosyltransferase enzyme.

46. The method according to claim 45, wherein said potential inhibitor is selected from a database.

47. The method according to claim 45, wherein said potential inhibitor is designed de novo.

48. The method according to claim 45, wherein said potential inhibitor is designed from a known inhibitor.

49. The method according to claim 45, wherein said step of employing said three-dimensional structure to design or select said potential inhibitor comprises the steps of:

(a) identifying chemical entities or fragments capable of associating with UDP-glycosyltransferase enzyme; and

(b) assembling the identified chemical entities or fragments into a single molecule to provide the structure of said potential inhibitor.

50. The method according to claim 45, wherein the potential inhibitor is a competitive inhibitor of mutant UDP-glycosyltransferase enzyme.

51. The method according to claim 45, wherein said potential inhibitor is a noncompetitive or uncompetitive inhibitor of mutant UDP-glycosyltransferase enzyme.

52. A model of a UDP-glycosyltransferase, wherein the model represents a three-dimensional structure that substantially conforms to the atomic coordinates of Table 1.

53. The model of claim 52, wherein the structure substantially conforms to the atomic coordinates and B-values represented by Table 1.

54. The model of claim 52, wherein the structure is monomeric.

55. The model of claim 52, wherein at least about 50% of the structure has an average root-mean-square deviation (RMDS) of less than about 2.5 Å for backbone atoms in secondary structure elements in each domain of the structure.

56. The model of claim 52, wherein the MurG protein comprises an amino acid sequence that is at least about 25% identical to the amino acid sequence of the *E. coli* MurG protein.

57. The model of claim 52, wherein the MurG protein comprises an amino acid sequence that is at least about 40% identical to the amino acid sequence of the *E. coli* MurG protein.

58. The model of claim 52, wherein the MurG protein comprises an amino acid sequence that is at least about 60% identical to the amino acid sequence of the *E. coli* MurG protein.

59. The model of claim 52, wherein the MurG protein comprises an amino acid sequence selected, from the group consisting of the amino acid sequence of a MurG protein from *Escherichia coli, Bacillus subtilis, Aquefex aeolicus, Borrelia burgdorferi, Chlamydia pneumoniae, Chlamydia trachomatis, Enterococcus faecais, Enterococcus hirae, Haemophilus influenzae, Helicobacter pylori J99, Helicobacter pylori, Afycobacterium tuberculosis, Porphyromonas gingivalis, Rickettsia prowazekii, Streptomyces coeticolor, Streptomyces collinus, Streptococcus pneumoniae, Synechocystis* sp. (strain PCC6803), *Thermotoga maritime,* and *Treponema pallidum,* a mutant of any of the amino acid sequences, and a variants of any of the amino acid sequences.

60. The model of claim 52, wherein the MurG protein comprises an amino acid sequence selected from the group consisting of the amino acid sequences of MurG proteins as deposited in the NCBI database and identified with Accession Nos. CAB51993, A71316, E70579, C71699, F70195, A43727, JC1275, BVECMG, CEECAM, O83535, Q9ZK59, CAB85280, AAF39020, BAA18775, AAD26629, CAB73295, P37585, Q9ZHA9, Q9ZHDC0, Q9ZBA5, Q9X4H4, Q9WY74, P74657, O06224, Q9Z702, O84766, O69552, O67238, O51708, O25770, O07670, O07109, P45065, CAB66324, AAC68356, AAF06830, P18579, P17443, P17952, P16457, P07862, AAE23178, AAD53936, CAA18668, CAA38869, CAA38868, CAA38867, CAA38866, AAD08196, BAA01453, BAA01455, BAA01454, AAD19042, CAA45558, CAA74235, AAD10537, AAD06652, AAC95450, CAA14869, AAC73201, AAC65509, AAC67113, AAC45636, CAB08640, AAC22793, AAC07193, BAA24357, CAB13395, BAA01355, AAB35538, 1904153C, 1808265B, 1808265A, CAA36866, CAA36869, CAA36868, CAA36867, CAA36776, and AAA99436.

61. The model of claim 52, wherein the MurG protein comprises an amino acid sequence obtained from an organism selected from the group consisting of bacteria, small pathogenic organisms, cyano bacteria, higher-order bacteria, spirochetes and thermal stable bacteria.

62. The model of claim 52, wherein the MurG protein comprises an amino acid sequence obtained from an organism selected from the group consisting of *Escherichia coli, Bacillus subtilis, Aquefex aeolicus, Borrelia burgdorferi, Chlamydia*

pneumoniae, Chlamydia trachomatis, Enterococcus faecais, Enterococcus hirae, Haemophilus influenzae, Helicobacter pylori J99, Helicobacter pylori, Mycobacterium tuberculosis, Porphyromonas gingivalis, Rickettsia prowazekii,Streptomyces coelicolor, Streptomyces collinus, Streptococcus pneumoniae, Synechocystis sp. (strain PCC6803), *Thermotoga marithne,* and *Treponema pallidum.*

63. The model of claim 52, wherein the MurG protein is a structural homologue of the *E. coli* MurG protein.

64. The model of claim 52, wherein the structure comprises an n-terminal and C-terminal domain connected by a covalent peptide linker, and wherein each domain has an alpha/beta fold.

65. The model of claim 52, wherein the RMSD is less than 2.5 Å over at least 80 aligned C-alpha atoms in each domain.

66. The model of claim 52, wherein the N-terminal domain comprises two glycine rich loops.

67. The model of claim 66, wherein the, amino acid sequence of the two glycine rich loops comprises GGTGGH and G-GGYVSG.

68. The model of claim 52, wherein the C-terminal domain comprises one glycine rich loop.

69. The model of claim 68, wherein the glycine rich loop comprises the amino acid sequence GGSQGAR or GGS-GAR.

70. The model of claim 52, wherein the atomic coordinates are generated by the method comprising the steps of:

(a) providing a MurG protein in crystalline form;

(b) generating an electron-density map of the crystalline MurG protein; and

(c) analyzing the electron-density map to produce the atomic coordinates.

71. The model of claim 70, wherein the crystalline MurG protein is produced by a method comprising the steps of:

(a) combining MurG protein with UDP-GlcNAc; and

(b) inducing crystal formation to produce said crystalline MurG protein.

72. The model of claim 70, wherein the crystalline MurG protein is produced by the hanging drop method in which MurG in buffer is at a concentration of at least 5 ug/ml and is combined with a reservoir solution and crystallizes.

73. The model of claim 72, wherein the buffer has a pH range from about 6.5 to about 9.0, and a buffer concentration range from about 10 mM to about 200 mM.

74. The model of 73, wherein the buffer is a Tris or a Hepes buffer, having a pH from about 7.0 to about,8.5.

75. The model of 74, wherein the buffer has a pH of about 7.9.

76. The model of claim 73, wherein the buffer further comprises at least one salt, chelating agent, or reducing agent.

77. The model of claim 72, wherein the reservoir solution has a pH range from about 5.0 to about 9.0 and the buffer concentration ranges from about 10 mM to about 1M.

78. The model of claim 77, wherein the reservoir solution further comprises at least one suitable precipitant, a detergent, and a reducing agent.

79. The model of claim 78, wherein the reservoir solution comprises a NaMES or sodium citrate buffer having a pH from about 6.0 to about 7.0.

80. The model of claim 79, wherein the buffer has a p14 of about 6.5.

81. The model of claim 78, wherein the precipitant is selected from the group consisting of ammonium sulfate and sodium potassium tartrate.

82. The model of 78, wherein the detergent is TritonX-100.

83. The model of 78, wherein the reducing agent is DTT, DTE or beta-mercaptoethanol.

84. The model of claim 71, wherein the MurG protein and the UDP-GlcNAc are in a 1:3 molar ratio.

85. The model of claim 71, wherein the buffer comprises 0.1 M NaMES, pH6.5, 0.9M $(NH_4)_2SO_4$,0.4% TRITON X-100®, and 10 mM dithiothreitol (DTT).

86. The model of claim 71, wherein the step of generating an electron-density map comprises analyzing the crystalline MurG protein by X-ray diffraction.

87. The model of claim 70, wherein the model is a computer image generated by a computer-readable medium encoded with a set of three-dimensional coordinates of the three-dimensional structure, wherein, using a graphical display software program, the three-dimensional coordinates create an electronic file that can be

visualized on a computer capable of representing the electronic file as a three-dimensional image.

88. A model of a donor nucleotide binding site of a UDP-glycosyltransferase (MurG) protein, wherein the model represents a three-dimensional structure that substantially conforms to the atomic coordinates of Table 4.

89. The model of claim 88, wherein the donor nucleotide binding site is located within the MurG C-terminal domain.

90. The model of claim 88, wherein the structure substantially conforms to the atomic coordinates and B-values of Table 4.

91. The model of claim 88, wherein at least about 50% of the structure has an average root-mean-square (RMSD) of less than about 2.5Å for the conserved amino acid residues for the donor nucleotide binding site of the *E. coli* MurG.

92. The model of claim 88, wherein the donor nucleotide binding site comprises an amino acid sequence that is at least about 70% identical to the conserved amino acid residues of the donor nucleotide binding site of *E. coli* MurG.

93. The model of claim 88, wherein the donor nucleotide binding site comprises an amino acid sequence that is at least about 80% identical to the conserved amino acid residues of the donor nucleotide binding site of the *E. coli* MurG.

94. The model of claim 88, wherein the donor nucleotide binding site comprises an amino acid sequence that is at least about 90% identical to the conserved amino acid residues of the donor nucleotide binding site, of the *E. coli* MurG.

95. The model of claim 88, wherein the donor nucleotide binding site comprises an amino acid sequence that is at least about 95% identical to the conserved amino acid residues of the donor nucleotide binding site of the *E. coli* MurG.

96. The model of claim 88, wherein the atomic coordinates are generated by a method comprising the steps of:

(a) providing a MurG protein in a crystalline form:

(b) generating an electron-density map of said crystalline MurG protein; and

(c) analyzing the electron-density map to produce the atomic coordinates.

97. The model of claim 88, wherein the model is a computer image generated by a computer-readable medium encoded with a set of three-dimensional coordinates of the three-dimensional structure, wherein, using a graphical display

software program, the three-dimensional coordinates create an electronic file that can be visualized on a computer capable of representing the electronic file as a three-dimensional image.

98. A model of an acceptor binding site of a UDP-glycosyltransferase (MurG) protein, wherein the model represents a three-dimensional structure that substantially conforms to the atomic coordinates of Table 5.

99. The model of claim 98, wherein the structure substantially conforms to the atomic coordinates and B-values of Table 5.

100. The model of claim 98, wherein at least about 50% of the structure has an average root-mean-square (RMSD) of less than about 1.5Å for the conserved amino acid residues in the acceptor binding site.

101. The model of claim 98, wherein the acceptor binding site comprises an amino acid sequence that is at least about 70% identical to the conserved amino acid residues of the acceptor binding site of *E. coli* MurG.

102. The model of claim 98, wherein the acceptor binding site comprises an amino acid sequence that is at least about 80% identical to the conserved amino acid residues of the acceptor binding site of *E. coli* MurG.

103. The model of claim 98, wherein the acceptor binding site comprises an amino acid sequence that is at least about 90% identical to the conserved amino acid residues of the *E. coli* MurG.

104. The model of claim 98, wherein the acceptor binding site comprises an amino acid sequence that is at least about 95% identical to the conserved amino acid residues of the acceptor binding site of the *E. coli* MurG.

105. The model of claim 98, wherein the acceptor binding site comprises an amino acid sequence that is at least about 70% identical to the amino acid sequence selected from the group consisting of *Escherichia coli, Bacillus subtilis, Aquefex aeolicus, Borrelia burgdorferi, Chlamydia pneumoniae, Chlamydia trachomatis, Enterococcus faecais, Enterococcus hirae, Haemophilus influenzae, Helicobacter pylorl J99, Helicobacter pylori, Mycobacterium tuberculosis, Porphyromonas gingivalis, Rickettsia prowazekii,Streptomyces coelicolor, Streptomyces collinus, Streptococcus pneumoniae, Synechocystis* sp. (strain PCC6803), *Thermotoga maritime,* and *Treponema pallidum.*

106. The model of claim 98, wherein the atomic coordinates are generated by the method comprising the steps of:

(a) providing a MurG protein in a crystalline form:

(b) generating an electron-density map of said crystalline MurG protein; and

(c) analyzing the electron-density map to produce the atomic coordinates.

107. The model of claim 98, wherein the model is a computer image generated by a computer-readable medium encoded with a set of three-dimensional coordinates of the three-dimensional structure, wherein, using a graphical display software program, the three-dimensional coordinates create an electronic file that can be visualized on a computer capable of representing the electronic file as a three-dimensional image.

108. A model of a membrane association site of a UDP-glycosyltransferase (MurG) protein, wherein the model represents a three-dimensional structure that substantially conforms to the atomic coordinates of Table 6.

109. The model of claim 108, wherein the structure substantially conforms to the atomic coordinates and B-values of Table 4.

110. The model of claim 108, wherein at least about 50% of the structure has an average root-mean-square (RMSD) of less than about 1.5Å for conserved amino acid residues in the *E. coli* membrane association site.

111. The model of claim 108, wherein the membrane association site comprises an amino acid sequence that is at least about 70% identical to the conserved amino acid residues of the membrane association site of *E. coli* MurG.

112. The model of claim M, wherein the membrane association site comprises an amino acid sequence that is at least about 80% identical to the conserved amino acid residues of the membrane association site of the *E. coli* MurG.

113. The model of claim 108, wherein the membrane association site comprises an amino acid sequence that is at least about 90% identical to the conserved amino acid residues of the membrane association site of the *E. coli* MurG.

114. The model of claim 108, wherein the membrane association site comprises an amino acid sequence that is at least about 95% identical to the conserved amino acid residues of a membrane association site of the *E. coli* MurG.

115. The model of claim 108, wherein the membrane association site comprises an amino acid sequence that is at least about 70% identical to the amino acid sequence from organisms selected from the group consisting of *Escherichia coli, Bacillus subtilis, Aquefex aeolicus, Borrelia burgdorferi, Chlamydia pneumoniae, Chlamydia trachomatis, Enterococcus faecais, Enterococcus hirae, Haemophilus influenzae, Helicobacter pylori J99, Helicobacter pylori, Mycobacterium tuberculosis, Porphyromonas gingivalis, Rickettsia prowazekii, Streptomyces coelicolor, Streptomyces collinus, Streptococcus pneumoniae, Synechocystis* sp. (strain PCC6803), *Thermotoga maritime,* and *Treponema pallidum.*

116. The model of claim 108, wherein the model is a computer image generated by a computer-readable medium encoded with a set of three-dimensional coordinates of the three-dimensional structure, wherein, using a graphical display software program, the three-dimensional coordinates create an electronic file that can be visualized on a computer capable of representing the electronic file as a three-dimensional image.

117. A computer-assisted method of structure based drug design of bioactive compounds, comprising the steps of:

(a) providing a model of a UDP-glycosyltransferase (MurG) protein or a donor nucleotide binding site, acceptor binding site or membrane association site; and

(b) designing a chemical compound using said model.

118. The method of claim 117, further comprising the step of synthesizing the chemical compound.

119. The method of claim 118, further comprising the step of evaluating the bioactivity of the synthesized chemical compound.

120. The method of claim 118, wherein the model of the UDP-glycosyltransferase (MurG) protein represents a three-dimensional structure comprising the atomic coordinates listed in Table 1.

121. The method of claim 118, wherein the model of the donor nucleotide binding site represents a three-dimensional structure comprising the atomic coordinates Table 4.

122. The method of claim 118, wherein the model of the acceptor binding site represents a three-dimensional structure comprising the atomic coordinates in Table 5.

123. The method of claim 118, wherein the model of the membrane association site represent a three-dimensional structure comprising the atomic coordinates in Table 6.

124. The method of claim 118, wherein the model comprises a computer image generated when the atomic coordinates listed in Table 1 are analyzed on a computer using a graphical display software program to create an electronic file of the image and visualizing the electronic file on a computer capable of representing the electronic file as a three-dimensional image.

125. The method of claim 118, wherein the step of designing comprises computational screening of one or more databases of chemical compounds in which the three-dimensional structure of said compounds are known.

126. The method of claim 125, further comprising interacting a compound identified by the screening step with the model by computer.

127. The method of claim 118, wherein the step of designing comprises directed drug design.

128. The method of claim 118, wherein the step of designing comprises random drug design.

129. The method of claim 118, wherein the step of designing comprises grid-based drug design.

130. The method of claim 118, wherein the step of designing comprises selecting compounds which are predicted to mimic the three-dimensional structure of the three-dimensional structure of the MurG protein.

131. The method of claim 118, wherein the step of designing comprises selecting compounds which are predicted to bind to the three-dimensional structure of the MurG protein.

132. The method of claim 118, wherein the bioactivity is selected from the group consisting of inhibiting binding of a nucleotide donor compound to the MurG protein, inhibiting binding of an acceptor compound to the MurG protein, or inhibiting association of the MurG Protein to a membrane.

133. A model of the three-dimensional, structure of a MurG protein , wherein the model is produced by the following method comprising the steps of:

(a) providing an amino acid sequence of a MurG protein and the amino acid sequence of the *Escherichia coli* MurG protein;

(b) identifying structurally conserved regions shared between the MurG protein and the *E. coli* MurG protein; and

(c) determining atomic coordinates for the MurG protein by assigning the structurally conserved regions of the MurG protein to a three-dimensional structure using a three-dimensional structure of the MurG protein which substantially conforms to the atomic coordinates represented in Table 1, to derive a model of the three-dimensional structure of the MurG protein amino acid sequence.

134. The model of claim 133, wherein the MurG protein amino acid sequence comprises the sequence of an amino acid sequence selected from the group consisting of the amino acid sequences of MurG proteins as deposited in the NCBI database and identified with Accession Nos. CAB51993, A71316, E70579, C71699, F70195, A43727, JC1275, BVECMG, CEECAM, O83535, Q9ZK59, CAB85280, AAF39020, BAA18775, AAD26629, CAB73295, P37585, Q9ZHA9, Q9ZHDC0, Q9ZBA5, Q9X4H4, Q9WY74, P74657, O06224, Q9Z702, O84766, O69552, O67238, O51708, O25770, O07670, O07109, P45065, CAB66324, AAC68356, AAF06830, P18579, P17443, P17952, P16457, P07862, AAE23178, AAD53936, CAA18668, CAA38869, CAA38868, CAA38867, CAA38866, AAD08196, BAA01453, BAA01455, BAA01454, AAD19042, CAA45558, CAA74235, AAD10537, AAD06652, AAC95450, CAA14869, AAC73201, AAC65509, AAC67113, AAC45636, CAB08640, AAC22793, AAC07193, BAA24357, CAB13395, BAA01355, AAB35538, 1904153C, 1808265B, 1808265A, CAA36866, CAA36869, CAA36868, CAA36867, CAA36776, and AAA99436.

135. A composition for inhibiting the activity of a glycosyltransferase comprising a compound that inhibits the activity of a glycosyltransferase, wherein the compound is identified by the method comprising the steps of:

(a) providing a three-dimensional structure of a MurG protein;

(b) using the three-dimensional structure of the MurG protein to design a chemical compound that inhibits activity of a glycosyltransferase;

(c) synthesizing the chemical compound; and

(d) evaluating the ability of the chemical compound to inhibit the activity of a glycosyltransferase.

136. The composition of claim 135, wherein the glycosyltransferase is a MurG protein.

137. The composition of claim 135, wherein the three-dimensional structure of the MurG protein substantially conforms to atomic coordinates represented by Table 1.

138. The composition of claim 135, wherein the compound is selected from the group consisting of an inorganic and an organic compound.

139. The composition of claim 135, wherein the compound is a substituted pyrimidine analogs.

140. The composition, of claim 135, wherein the compound is selected from the group consisting of an analog of a MurG protein, a substrate analog of a MurG protein, a donor molecule analog of a MurG protein, and a membrane analog of a MurG protein.

141. The composition of claim 135, further comprising a component selected from the group consisting of an excipient an adjuvant, and a carrier.

142. A composition for stimulating the activity of a glycosyltransferase comprising a compound that stimulates the activity of a glycosyltransferase, wherein the compound is identified by the method comprising the steps of:

(a) providing a three-dimensional structure of a MurG protein;

(b) using the three-dimensional structure of the MurG protein to design a chemical compound that inhibits activity of a glycosyltransferase;

(c) synthesizing the chemical compound; and

(d) evaluating the ability of the chemical compound to stimulate the activity of a glycosyltransferase.

143. A method to determine a three-dimensional structure of a MurG protein comprising the steps of:

(a) providing an amino acid sequence of a MurG protein, wherein the three-dimensional structure of the MurG protein is not known;

(b) analyzing the pattern of folding of the amino acid sequence in a three-dimensional conformation by fold recognition; and

(c) comparing the pattern of folding of the MurG protein amino acid sequence with the three-dimensional structure of the *E. coli* MurG protein, wherein the three-dimensional structure of the *E. coli* MurG protein substantially conforms to the atomic coordinates represented in Table 1.

144. A method to derive a model of the three-dimensional structure of a MurG protein comprising the steps of:

(a) providing an amino acid sequence of a MurG protein;

(b) identifying structurally conserved regions shared between the MurG protein and the *E. coli* MurG protein;

(c) determining atomic coordinates for the MurG protein structure by assigning the structurally conserved regions of the MurG protein to a three-dimensional structure using a three-dimensional structure of the *E. coli* MurG protein based on atomic coordinates represented in Table 1 to derive a model of the three-dimensional structure of the MurG protein amino acid sequence.

145. The method of claim 144, further comprising assigning atomic coordinates for side chains of said MurG protein by determining sterically allowable positions using a library of rotamers.

146. A method to derive a three-dimensional structure of a crystallized MurG protein comprising the steps of:

(a) comparing the Patterson function of a crystallized MurG protein with the Patterson function of crystalline *E. coli* MurG protein to produce an electron-density map of the crystallized MurG protein; and

(b) analyzing the electron-density map to produce the three-dimensional structure of the crystallized MurG protein.

147. The method of claim 146, further comprising the step of rotating the Patterson function of the crystallized MurG protein on the Patterson function of the crystalline E coli MurG protein to determine the correct orientation of the crystallized MurG protein in a crystal of said crystallized MurG protein to identify the initial phases of the crystallized MurG protein.

148. The method of claim 146, further comprising the step of electronically stimulating the three-dimensional structure of the crystallized MurG protein to derive a computer image of the three-dimensional structure of the crystallized MurG protein.

ABSTRACT OF THE DISCLOSURE

The present invention relates to crystals of the *Escherichia coli* MurG, a membrane-associated UDP-glycosyltransferase involved in peptidoglycan biosynthesis. The present invention also relates to three-dimensional atomic coordinates of the MurG protein, three-dimensional structures of the protein, and images thereof. The present invention also relates to the atomic coordinates and three-dimensional structures of the α-carbon backbone and of the α-carbon backbone and conserved amino acid residue sidechains of the MurG protein and images thereof. The present invention further relates to three-dimensional atomic coordinates of the donor nucleotide binding site, the acceptor binding site, and the membrane association site of the MurG protein, three-dimensional structures of the binding domains, and images thereof. The present invention also relates to computer readable media encoded with sets of the three-dimensional coordinates described herein. The present invention relates to methods of crystallizing MurG proteins. The present invention relates to models of three-dimensional structures of UDP-glycosyltransferases and, in particular, MurG proteins, based on the three-dimensional structure of crystals of the *Escherichia coli* MurG. The present invention also relates to models of the three-dimensional structures of the α-carbon backbone and the α-carbon backbone and conserved amino acid residue sidechains of UDP-glycosyltransferases and MurG proteins and of the binding sites thereof. The present invention also relates to methods of drug design using models of this invention, the compounds identified using models of the present invention that bind, inhibit or stimulate UDP-glycosyltransferases or MurG proteins, and compositions comprising compounds identified using the models of this invention for therapeutic or diagnostic uses. Also, the present invention relates to methods of making models of the present invention.